

Technical Disclosure Commons

Defensive Publications Series

October 2021

Predicted Binders for Various Protein Targets from Machine Learning Applied to Affinity Screening Data

Anonymous

Follow this and additional works at: https://www.tdcommons.org/dpubs_series

Recommended Citation

Anonymous, "Predicted Binders for Various Protein Targets from Machine Learning Applied to Affinity Screening Data", Technical Disclosure Commons, (October 19, 2021)
https://www.tdcommons.org/dpubs_series/4667



This work is licensed under a [Creative Commons Attribution 4.0 License](https://creativecommons.org/licenses/by/4.0/).

This Article is brought to you for free and open access by Technical Disclosure Commons. It has been accepted for inclusion in Defensive Publications Series by an authorized administrator of Technical Disclosure Commons.

Predicted Binders for Various Protein Targets from Machine Learning Applied to Affinity Screening Data

Anonymous

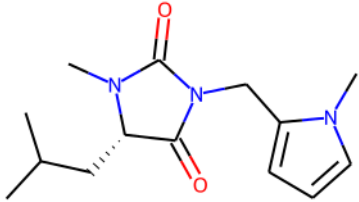
October 18, 2021

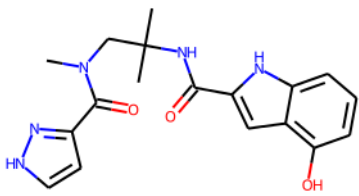
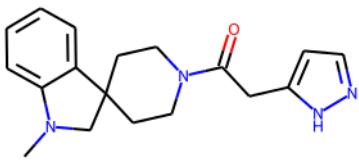
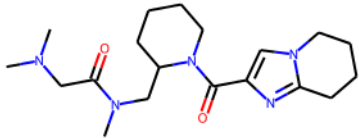
Abstract

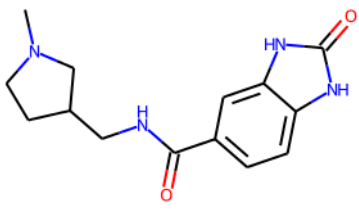
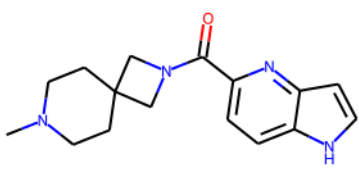
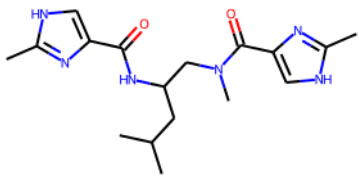
We used datasets from affinity screening to train machine learning models. The models were then used to rank compounds from commercially available compound collections to generate the following lists of predicted binders. The following lists of compounds were predicted by the ML model to be binders for the protein targets: CORO1A, RFWD3, MID1, WDR91, TRIM9.

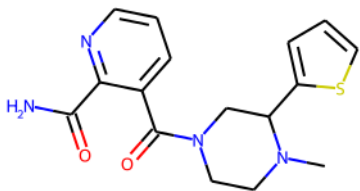
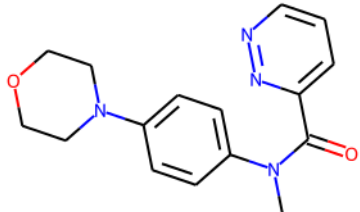
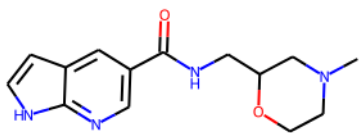
1 CORO1A

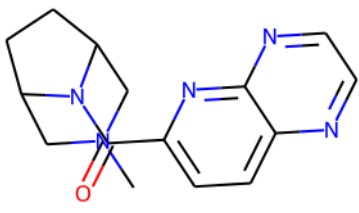
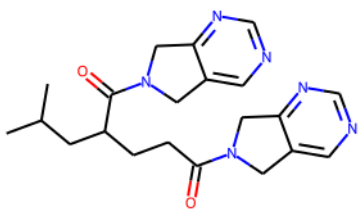
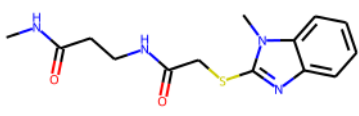
UniProtKB entry P31146

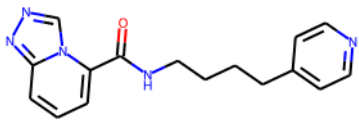
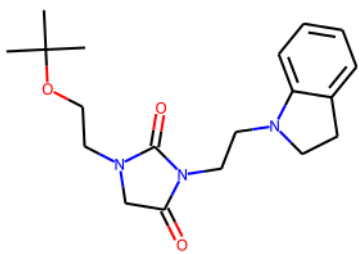
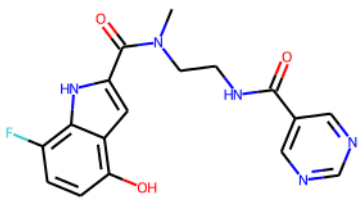
Chemical Structure	SMILES	Vendor
	<chem>CC(C)C[C@H]1C(=O)N(Cc2cccn2C)C(=O)N1C</chem>	ENAMINE Z2205790339

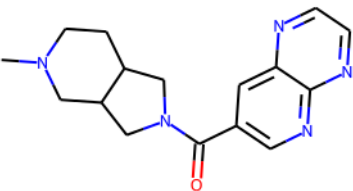
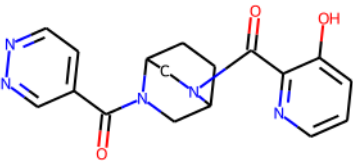
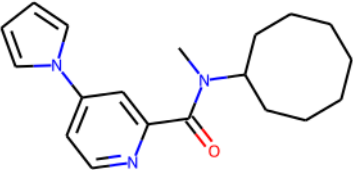
Chemical Structure	SMILES	Vendor
	<chem>CN(CC(C)(C)NC(=O)c1c c2c(O)cccc2[nH]1)C(=O)c1cc[nH]n1</chem>	ENAMINE PV-003293635609
	<chem>CN1CC2(CCN(C(=O)Cc3c cn[nH]3)CC2)c2cccc21</chem>	ENAMINE Z3893171369
	<chem>CN(C)CC(=O)N(C)CC1CC CCN1C(=O)c1cn2c(n1)CCCC2</chem>	ENAMINE PV-003923621773

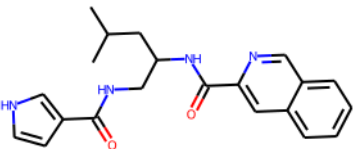
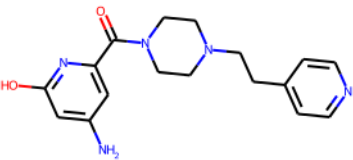
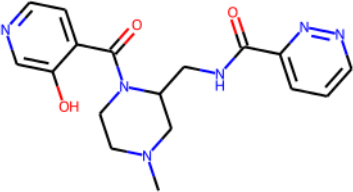
Chemical Structure	SMILES	Vendor
	<chem>CN1CCC(CNC(=O)c2ccc3[nH]c(=O)[nH]c3c2)C1</chem>	ENAMINE Z1174140371
	<chem>CN1CCC2(CC1)CN(C(=O)c1ccc3[nH]ccc3n1)C2</chem>	ENAMINE Z3589577949
	<chem>Cc1nc(C(=O)NC(CC(C)C)CN(C)C(=O)c2c[nH]c(C)n2)c[nH]1</chem>	ENAMINE Z1535303095

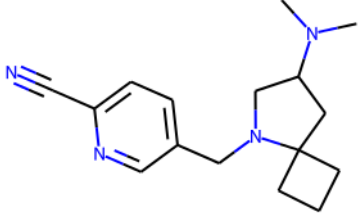
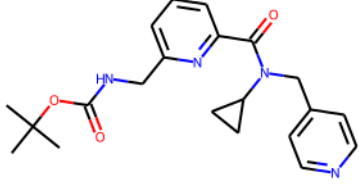
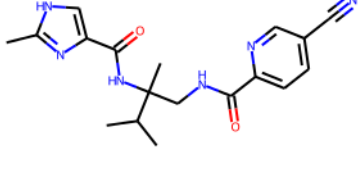
Chemical Structure	SMILES	Vendor
	<chem>CN1CCN(C(=O)c2ccnc2C(N)=O)CC1c1cccs1</chem>	ENAMINE Z4472168295
	<chem>CN(C(=O)c1cccn1)c1ccc(N2CCOCC2)cc1</chem>	ENAMINE Z2817978660
	<chem>CN1CCOC(CNC(=O)c2cnc3[nH]ccc3c2)C1</chem>	ENAMINE Z2267568206

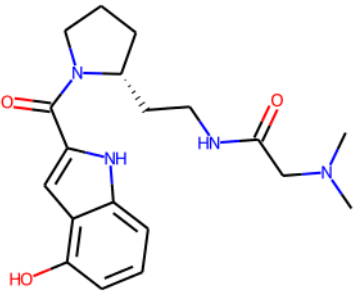
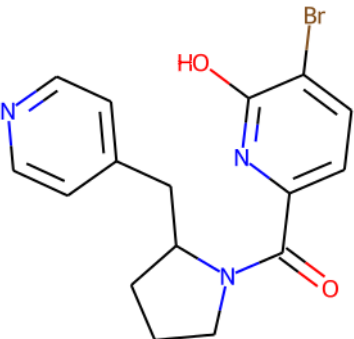
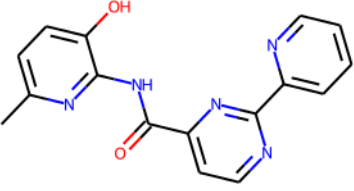
Chemical Structure	SMILES	Vendor
	<chem>CN1CC2CCC(C1)N2C(=O)c1ccc2ncnc2n1</chem>	ENAMINE Z2916154040
	<chem>CC(C)CC(CCC(=O)N1Cc2cncnc2C1)C(=O)N1Cc2cncnc2C1</chem>	ENAMINE Z2499946558
	<chem>CNC(=O)CCNC(=O)CSc1nc2ccccc2n1C</chem>	ENAMINE Z845587576

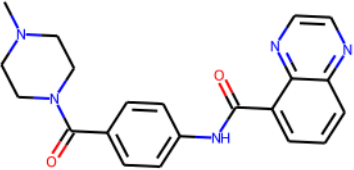
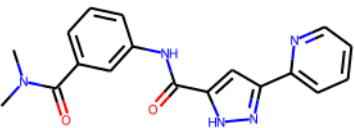
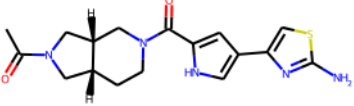
Chemical Structure	SMILES	Vendor
	<chem>O=C(NCCCCc1cncc1)c1cccc2nncn12</chem>	ENAMINE Z4227276250
	<chem>CC(C)(C)OCCN1CC(=O)N(CCN2CCc3cccc32)C1=O</chem>	ENAMINE Z3878761145
	<chem>CN(CCNC(=O)c1cncc1)C(=O)c1cc2c(O)ccc(F)c2[nH]1</chem>	ENAMINE PV-003298197704

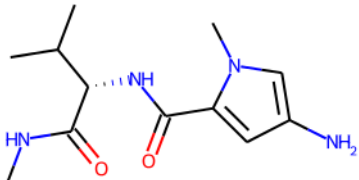
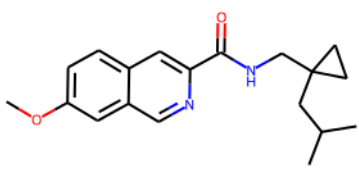
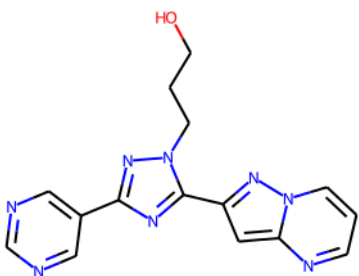
Chemical Structure	SMILES	Vendor
	<chem>CN1CCC2CN(C(=O)c3cnc4ncnc4c3)CC2C1</chem>	ENAMINE Z2184430865
	<chem>O=C(c1ccnnc1)N1CC2CC1CN2C(=O)c1ncccc1O</chem>	ENAMINE PV-000244941565
	<chem>CN(C(=O)c1cc(-n2cccc2)ccn1)C1CCCCCCC1</chem>	ENAMINE Z2130387712

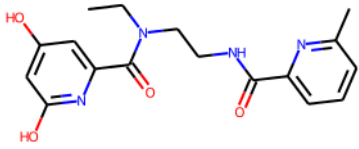
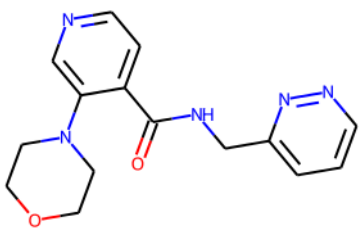
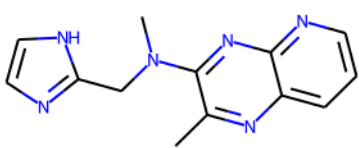
Chemical Structure	SMILES	Vendor
	<chem>CC(C)CC(CNC(=O)c1cc[nH]c1)NC(=O)c1cc2ccccc2cn1</chem>	ENAMINE PV-004119223070
	<chem>Nc1cc(O)nc(C(=O)N2CCN(CCc3ccncc3)CC2)c1</chem>	ENAMINE Z4293422948
	<chem>CN1CCN(C(=O)c2ccncc2O)C(CNC(=O)c2cccn2)C1</chem>	ENAMINE PV-002798568890

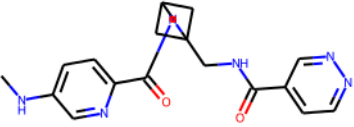
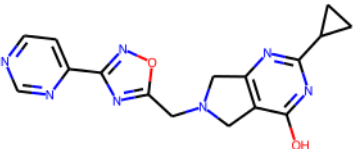
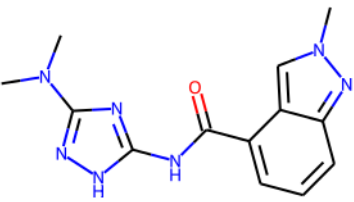
Chemical Structure	SMILES	Vendor
	<chem>CN(C)C1CN(Cc2ccc(C#N)nc2)C2(CCC2)C1</chem>	ENAMINE Z3488980916
	<chem>CC(C)(C)OC(=O)NCc1ccc(cc(C(=O)N(Cc2ccncc2)C2CC2)n1</chem>	ENAMINE Z4404929830
	<chem>Cc1nc(C(=O)NC(C)(C)NC(=O)c2ccc(C#N)cn2)C(C)C)c[nH]1</chem>	ENAMINE PV-003129758768

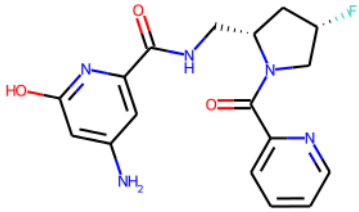
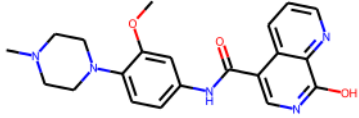
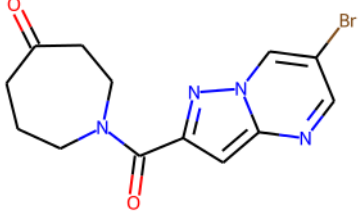
Chemical Structure	SMILES	Vendor
	<chem>CN(C)CC(=O)NCC[C@H]1</chem> <chem>CCCN1C(=O)c1cc2c(O)cccc2[nH]1</chem>	ENAMINE PV-003563472334
	<chem>O=C(c1ccc(Br)c(O)n1)</chem> <chem>N1CCCC1Cc1ccncc1</chem>	ENAMINE Z4294902097
	<chem>Cc1ccc(O)c(NC(=O)c2ccnc(-</chem> <chem>c3cccn3)n2)n1</chem>	ENAMINE PV-002578625288

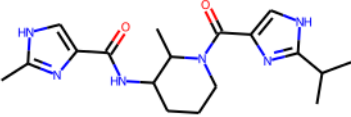
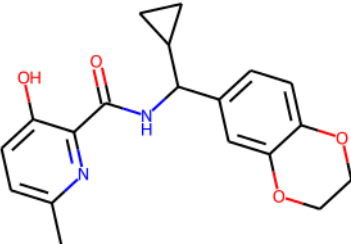
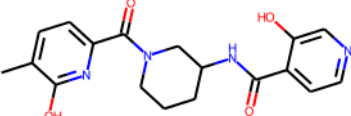
Chemical Structure	SMILES	Vendor
	<chem>CN1CCN(C(=O)c2ccc(NC(=O)c3cccc4ncnc34)cc2)CC1</chem>	ENAMINE Z1666148338
	<chem>CN(C)C(=O)c1cccc(NC(=O)c2cc(-c3cccn3)n[nH]2)c1</chem>	ENAMINE PV-002828407782
	<chem>CC(=O)N1C[C@H]2CCN(C(=O)c3cc(-c4csc(N)n4)c[nH]3)C[C@H]2C1</chem>	ENAMINE PV-003776180300

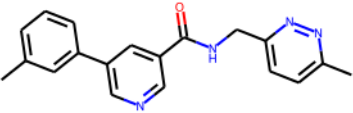
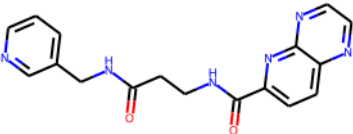
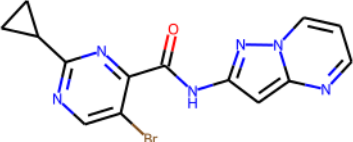
Chemical Structure	SMILES	Vendor
	<chem>CNC(=O)[C@H](NC(=O)c1cc(N)cn1C)C(C)C</chem>	ENAMINE Z4213245796
	<chem>COc1ccc2cc(C(=O)NCC3(CC(C)C)CC3)ncc2c1</chem>	ENAMINE PV-002902847074
	<chem>OCCCn1nc(-c2cncnc2)nc1-c1cc2ncccn2n1</chem>	ENAMINE PV-003782591780

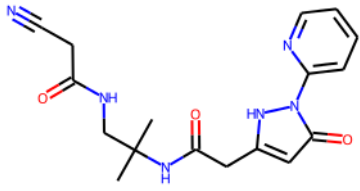
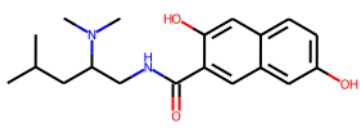
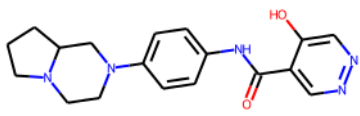
Chemical Structure	SMILES	Vendor
	<chem>CCN(CCNC(=O)c1cccc(C)n1)C(=O)c1cc(O)cc(O)n1</chem>	ENAMINE PV-002919288127
	<chem>O=C(NCc1cccn1)c1ccncc1N1CCOCC1</chem>	ENAMINE Z2776078044
	<chem>Cc1nc2cccnc2nc1N(C)Cc1ncc[nH]1</chem>	ENAMINE PV-002573605879

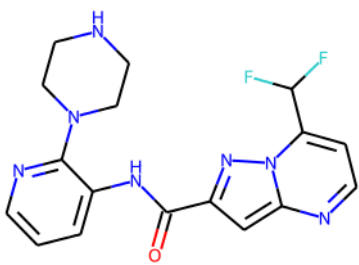
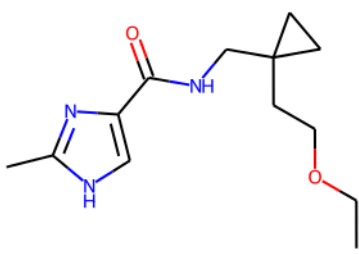
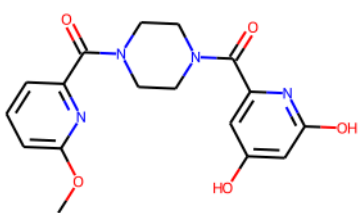
Chemical Structure	SMILES	Vendor
	<chem>CNc1ccc(C(=O)N2CC3CC2(CNC(=O)c2ccnnc2)C3)nc1</chem>	ENAMINE PV-003276001467
	<chem>Oc1nc(C2CC2)nc2c1CN(Cc1nc(-c3ccnnc3)no1)C2</chem>	ENAMINE PV-002202926363
	<chem>CN(C)c1n[nH]c(NC(=O)c2ccccc3nn(C)cc23)n1</chem>	ENAMINE PV-003689221177

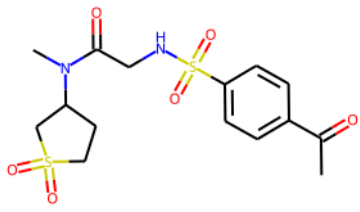
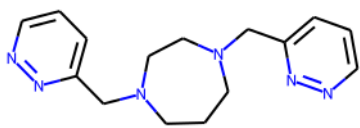
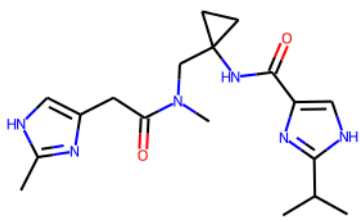
Chemical Structure	SMILES	Vendor
	<chem>Nc1cc(O)nc(C(=O)NC[C@@H]2C[C@H](F)CN2C(=O)c2cccn2)c1</chem>	ENAMINE PV-003154767005
	<chem>COc1cc(NC(=O)c2cnc(O)c3ncccc23)ccc1N1CCN(C)CC1</chem>	ENAMINE Z4475512653
	<chem>O=C1CCCN(C(=O)c2cc3ncc(Br)cn32)CC1</chem>	ENAMINE Z3633083788

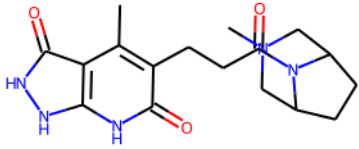
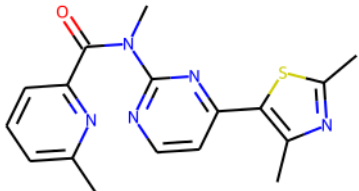
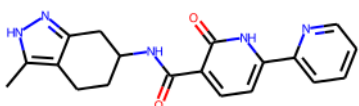
Chemical Structure	SMILES	Vendor
	<chem>Cc1nc(C(=O)NC2CCCN(C(=O)c3c[nH]c(C(C)C)n3)C2C)c[nH]1</chem>	ENAMINE PV-002793506938
	<chem>Cc1ccc(O)c(C(=O)NC(c2ccc3c(c2)OCCO3)C2CC2)n1</chem>	ENAMINE PV-003856804679
	<chem>Cc1ccc(C(=O)N2CCCC(NC(=O)c3ccncc3O)C2)nc1O</chem>	ENAMINE PV-003351052315

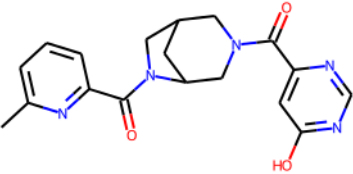
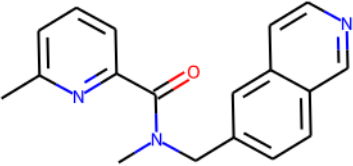
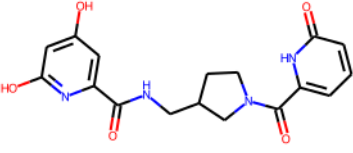
Chemical Structure	SMILES	Vendor
	<chem>Cc1cccc(-c2cncc(C(=O)NCc3ccc(C)nn3)c2)c1</chem>	ENAMINE PV-003047117638
	<chem>O=C(CCNC(=O)c1ccc2ncnc2n1)NCc1ccnc1</chem>	ENAMINE Z1982237108
	<chem>O=C(Nc1cc2ncccn2n1)c1nc(C2CC2)ncc1Br</chem>	ENAMINE PV-002768122753

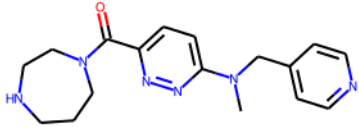
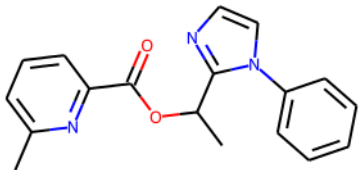
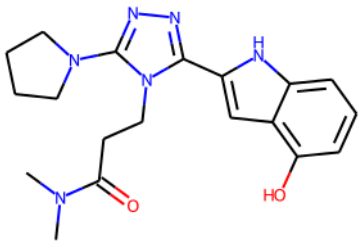
Chemical Structure	SMILES	Vendor
	<chem>CC(C)(CNC(=O)CC#N)NC(=O)Cc1cc(=O)n(-c2cccn2)[nH]1</chem>	ENAMINE PV-003316619769
	<chem>CC(C)CC(CNC(=O)c1cc2cc(O)ccc2cc1O)N(C)C</chem>	ENAMINE PV-003007601851
	<chem>O=C(Nc1ccc(N2CCN3CCCC3C2)cc1)c1cnnc1O</chem>	ENAMINE Z3053881525

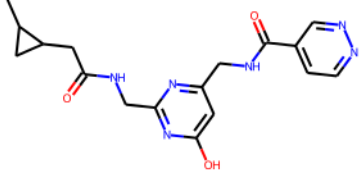
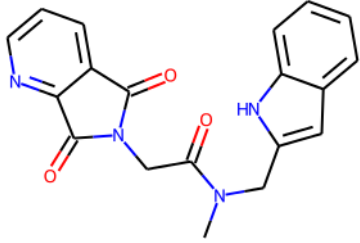
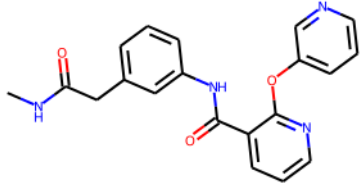
Chemical Structure	SMILES	Vendor
	<chem>O=C(Nc1ccccc1N1CCNCC1)c1cc2nccc(C(F)F)n2n1</chem>	ENAMINE Z4213987495
	<chem>CCOCCC1(CNC(=O)c2c[nH]c(C)n2)CC1</chem>	ENAMINE Z1502281196
	<chem>COc1cccc(C(=O)N2CCN(C(=O)c3cc(O)cc(O)n3)CC2)n1</chem>	ENAMINE PV-002956603534

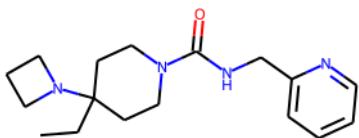
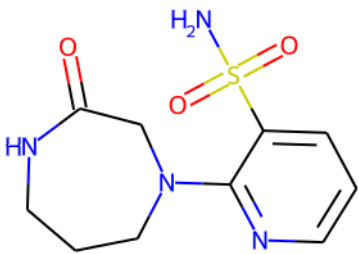
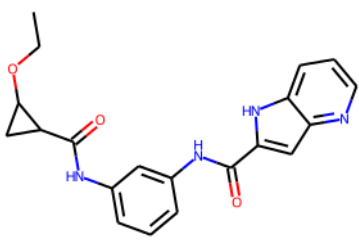
Chemical Structure	SMILES	Vendor
	<chem>CC(=O)c1ccc(S(=O)(=O)NCC(=O)N(C)C2CCS(=O)(=O)C2)cc1</chem>	ENAMINE Z183997408
	<chem>c1cnnc(CN2CCCN(Cc3ccnnc3)CC2)c1</chem>	ENAMINE Z4400420042
	<chem>Cc1nc(CC(=O)N(C)CC2(NC(=O)c3c[nH]c(C(C)C)n3)CC2)c[nH]1</chem>	ENAMINE PV-003831937479

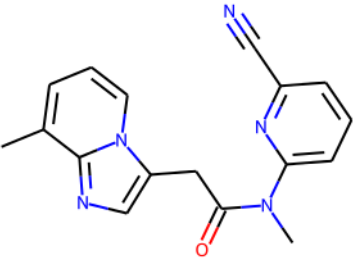
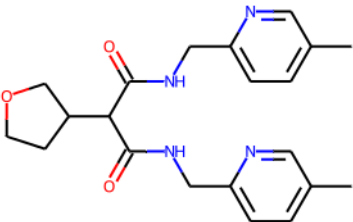
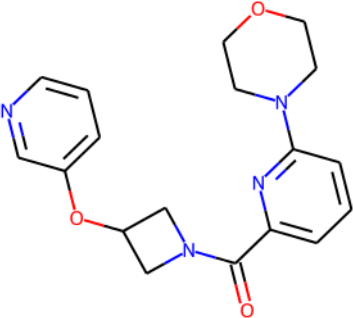
Chemical Structure	SMILES	Vendor
	<chem>Cc1c(CCC(=O)N2C3CCC2CN(C)C3)c(=O)[nH]c2[nH][nH]c(=O)c12</chem>	ENAMINE PV-003201753903
	<chem>Cc1cccc(C(=O)N(C)c2nccc(-c3sc(C)nc3C)n2)n1</chem>	ENAMINE PV-002414341832
	<chem>Cc1[nH]nc2c1CCC(NC(=O)c1ccc(-c3cccn3)[nH]c1=O)C2</chem>	ENAMINE PV-003883700688

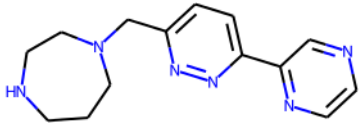
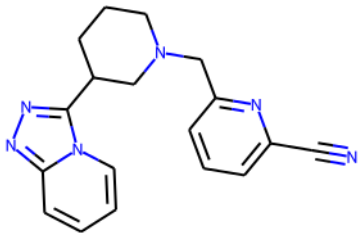
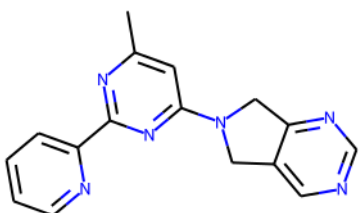
Chemical Structure	SMILES	Vendor
	<chem>Cc1cccc(C(=O)N2CC3CC2CN(C(=O)c2cc(O)ncn2)C3)n1</chem>	ENAMINE PV-002939889041
	<chem>Cc1cccc(C(=O)N(C)Cc2ccc3cnccc3c2)n1</chem>	ENAMINE PV-002480373596
	<chem>O=C(NCC1CCN(C(=O)c2ccc(=O)[nH]2)C1)c1cc(O)cc(O)n1</chem>	ENAMINE PV-003011275888

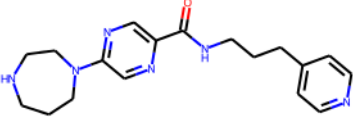
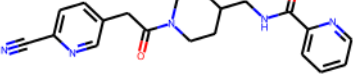
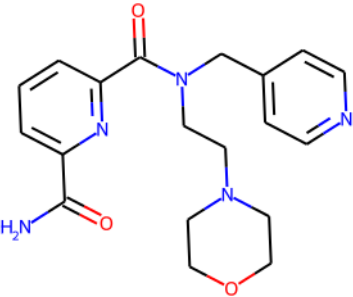
Chemical Structure	SMILES	Vendor
	<chem>CN(Cc1ccncc1)c1ccc(C(=O)N2CCCNCC2)nn1</chem>	ENAMINE Z4080842545
	<chem>Cc1cccc(C(=O)OC(C)c2nccn2-c2ccccc2)n1</chem>	ENAMINE Z2073808890
	<chem>CN(C)C(=O)CCN1c(-c2c3c(O)cccc3[nH]2)nnc1N1CCCC1</chem>	ENAMINE Z3181054939

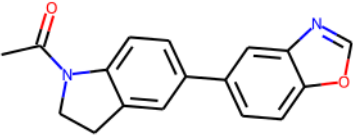
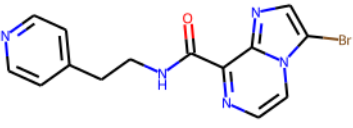
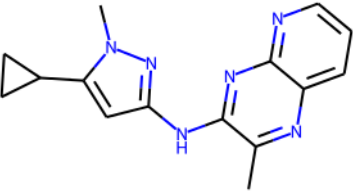
Chemical Structure	SMILES	Vendor
	<chem>CC1CC1CC(=O)NCc1nc(O)cc(CNC(=O)c2ccnnc2)n1</chem>	ENAMINE PV-001237846765
	<chem>CN(Cc1cc2cccc2[nH]1)C(=O)CN1C(=O)c2ccnnc2C1=O</chem>	ENAMINE Z1368695063
	<chem>CNC(=O)Cc1cccc(NC(=O)c2ccnnc2Oc3ccnnc3)c1</chem>	ENAMINE PV-003924237678

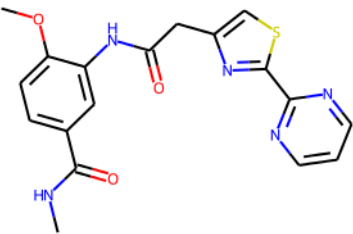
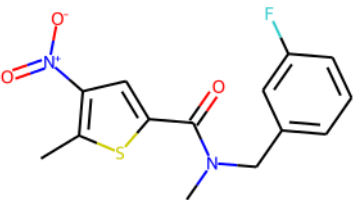
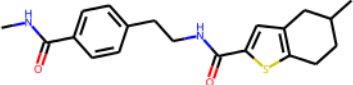
Chemical Structure	SMILES	Vendor
	<chem>CCC1(N2CCC2)CCN(C(=O)NCc2cccn2)CC1</chem>	ENAMINE Z2864010134
	<chem>NS(=O)(=O)c1cccn1N1CCCNC(=O)C1</chem>	ENAMINE Z1190326903
	<chem>CCOC1CC1C(=O)Nc1cccc(NC(=O)c2cc3ncccc3[nH]2)c1</chem>	ENAMINE PV-004064378491

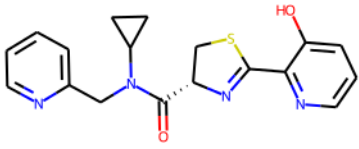
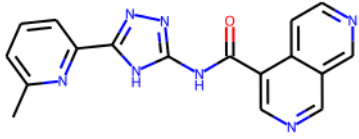
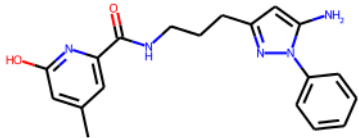
Chemical Structure	SMILES	Vendor
	<chem>Cc1cccn2c(CC(=O)N(C)c3cccc(C#N)n3)cnc12</chem>	ENAMINE PV-002517978295
	<chem>Cc1ccc(CNC(=O)C(C(=O)NCC2cccc(C)cn2)C2CCOC2)nc1</chem>	ENAMINE Z4106229274
	<chem>O=C(c1cccc(N2CCOCC2)n1)N1CC(Oc2cccn2)C1</chem>	ENAMINE Z4771488118

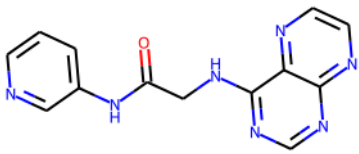
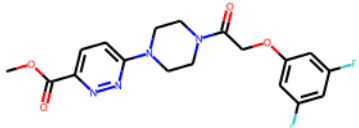
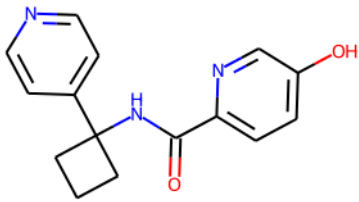
Chemical Structure	SMILES	Vendor
	<chem>c1cnc(-c2ccc(CN3CCCNCC3)nn2)cn1</chem>	ENAMINE Z4083029873
	<chem>N#Cc1cccc(CN2CCCC(c3nnc4cccn34)C2)n1</chem>	ENAMINE Z2824660286
	<chem>Cc1cc(N2Cc3cncnc3C2)nc(-c2cccn2)n1</chem>	ENAMINE PV-002475005542

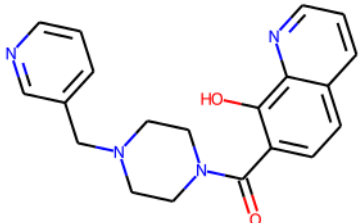
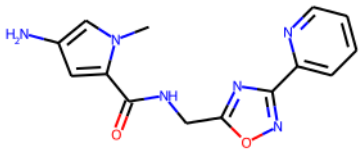
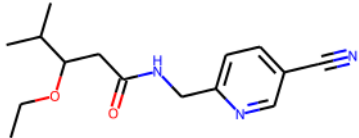
Chemical Structure	SMILES	Vendor
	<chem>O=C(NCCCC1CCNCC1)C1CNC(N2CCCCNCC2)CN1</chem>	ENAMINE Z3522532411
	<chem>N#Cc1ccc(CC(=O)N2CCC(CNC(=O)c3ccccc3)CC2)cn1</chem>	ENAMINE Z2708242183
	<chem>NC(=O)c1ccc(C(=O)N(CCN2CCOCC2)Cc2ccncc2)n1</chem>	ENAMINE Z1638858289

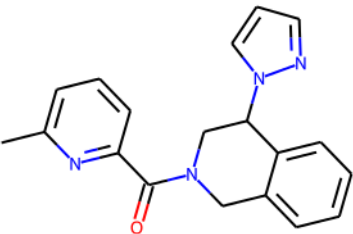
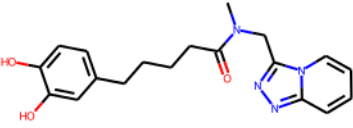
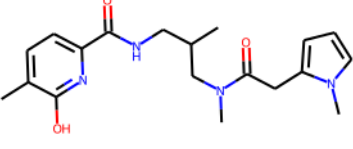
Chemical Structure	SMILES	Vendor
	<chem>CC(=O)N1CCc2cc(-c3ccc4ocnc4c3)ccc21</chem>	ENAMINE PV-002764883199
	<chem>O=C(NCCc1ccncc1)c1ncn2c(Br)cnc12</chem>	ENAMINE Z1570239318
	<chem>Cc1nc2cccnc2nc1Nc1cc(C2CC2)n(C)n1</chem>	ENAMINE Z3392381608

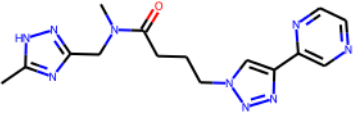
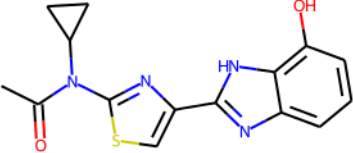
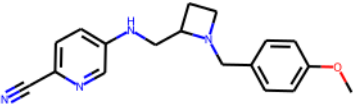
Chemical Structure	SMILES	Vendor
	<chem>CNC(=O)c1ccc(OC)c(NC(=O)Cc2csc(-c3ncccn3)n2)c1</chem>	ENAMINE Z772120498
	<chem>Cc1sc(C(=O)N(C)Cc2cc(F)c2)cc1[N+](=O)[O-]</chem>	ENAMINE Z336631798
	<chem>CNC(=O)c1ccc(CCNC(=O)c2cc3c(s2)CCC(C)C3)cc1</chem>	ENAMINE PV-002502373218

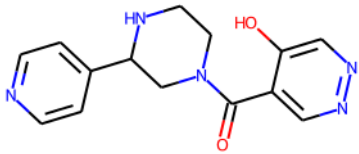
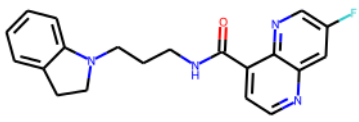
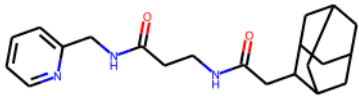
Chemical Structure	SMILES	Vendor
	<chem>O=C([C@@H]1CSC(c2ncc cc2O)=N1)N(Cc1cccn1)C1CC1</chem>	ENAMINE Z4315963518
	<chem>Cc1cccc(-c2nnc(NC(=O)c3cncc4cnccc34)[nH]2)n1</chem>	ENAMINE PV-002854630287
	<chem>Cc1cc(O)nc(C(=O)NCCCc2cc(N)n(- c3ccccc3)n2)c1</chem>	ENAMINE Z2212975945

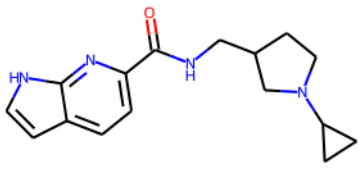
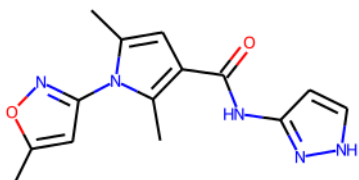
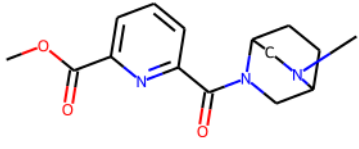
Chemical Structure	SMILES	Vendor
	<chem>O=C(CNc1ncnc2ncnc12)Nc1cccc1</chem>	ENAMINE Z1502752100
	<chem>COC(=O)c1ccc(N2CCN(C(=O)COc3cc(F)cc(F)c3)CC2)nn1</chem>	ENAMINE Z2174470921
	<chem>O=C(NC1(c2ccncc2)CCC1)c1ccc(O)cn1</chem>	ENAMINE Z3358794125

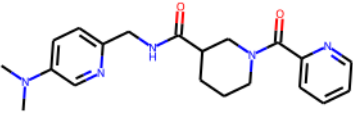
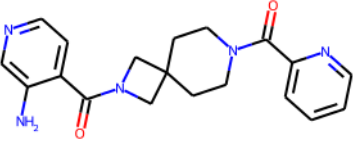
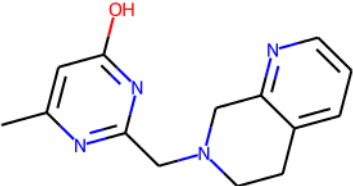
Chemical Structure	SMILES	Vendor
	<chem>O=C(c1ccc2cccnc2c1O)N1CCN(Cc2cccnc2)CC1</chem>	ENAMINE Z3467318279
	<chem>Cn1cc(N)cc1C(=O)NCc1nc(-c2cccn2)no1</chem>	ENAMINE PV-003134831876
	<chem>CCOC(CC(=O)NCc1ccc(C#N)cn1)C(C)C</chem>	ENAMINE Z1767448356

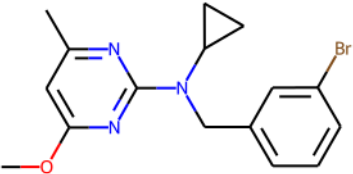
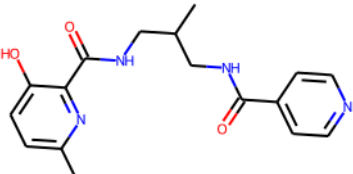
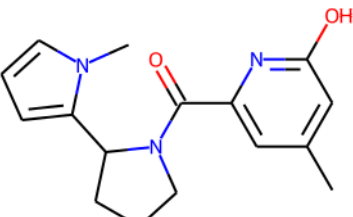
Chemical Structure	SMILES	Vendor
	<chem>Cc1cccc(C(=O)N2Cc3ccccc3C2)n1</chem>	ENAMINE Z1228027503
	<chem>CN(Cc1nnc2ccccc12)C(=O)CCCCc1ccc(O)c(O)c1</chem>	ENAMINE Z4306675928
	<chem>Cc1ccc(C(=O)NCC(C)CN(C)C(=O)Cc2cccn2C)nc1O</chem>	ENAMINE PV-003836592790

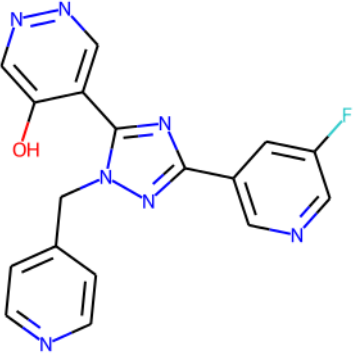
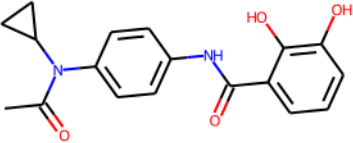
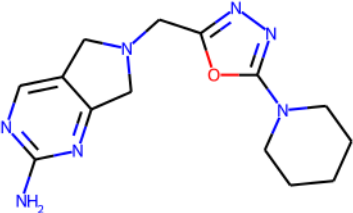
Chemical Structure	SMILES	Vendor
	<chem>Cc1nc(CN(C)C(=O)CCCN2cc(-c3cncn3)nn2)n[nH]1</chem>	ENAMINE PV-003893793487
	<chem>CC(=O)N(c1nc(-c2nc3c(O)ccc(O)c3[nH]2)cs1)C1CC1</chem>	ENAMINE Z3492834962
	<chem>COc1ccc(CN2CCC2CNc2cnc(C#N)nc2)cc1</chem>	ENAMINE Z2700645778

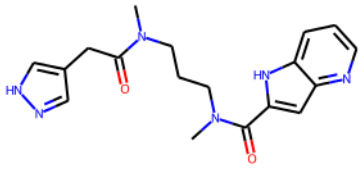
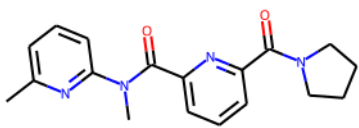
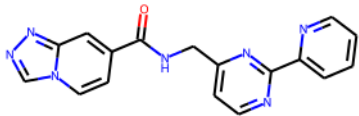
Chemical Structure	SMILES	Vendor
	<chem>O=C(c1cnccc1O)N1CCNC(c2ccncc2)C1</chem>	ENAMINE Z3051722650
	<chem>O=C(NCCCN1CCc2ccccc21)c1ccnc2cc(F)cnc12</chem>	ENAMINE Z2066688913
	<chem>O=C(CCNC(=O)CC1C2CC3CC(C2)CC1C3)NCc1cccn1</chem>	ENAMINE Z2480657463

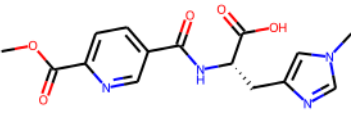
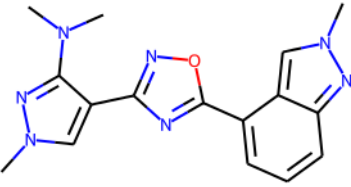
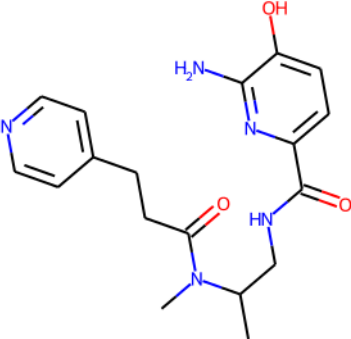
Chemical Structure	SMILES	Vendor
	<chem>O=C(NCC1CCN(C2CC2)C1)c1ccc2cc[nH]c2n1</chem>	ENAMINE Z1625130536
	<chem>Cc1cc(-n2c(C)cc(C(=O)Nc3cc[nH]n3)c2C)no1</chem>	ENAMINE Z1023224178
	<chem>COC(=O)c1cccc(C(=O)N2CC3CCC2CN3C)n1</chem>	ENAMINE Z4221898723

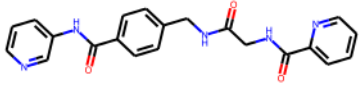
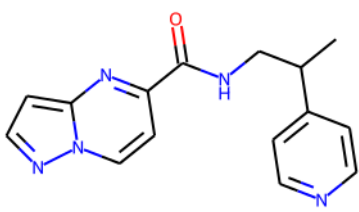
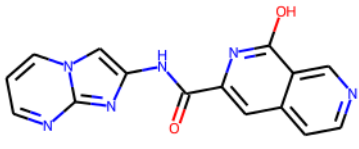
Chemical Structure	SMILES	Vendor
	<chem>CN(C)c1ccc(CNC(=O)C2CCCCC2C(=O)c3ccccn3)C2)nc1</chem>	ENAMINE Z4656535879
	<chem>Nc1enccc1C(=O)N1CC2(CCN(C(=O)c3ccccn3)CC2)C1</chem>	ENAMINE PV-002711917358
	<chem>Cc1cc(O)nc(CN2CCc3ccnc3C2)n1</chem>	ENAMINE Z4297286546


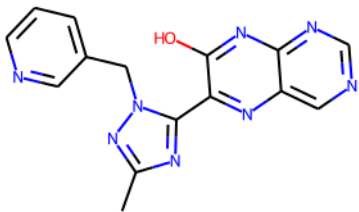
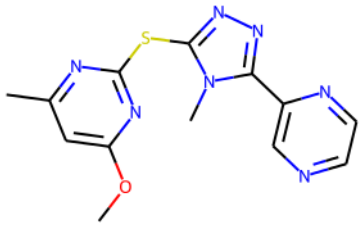
Chemical Structure	SMILES	Vendor
	<chem>COc1cc(C)nc(N(Cc2ccc(Br)cc2)CC2)cn1</chem>	ENAMINE PV-002494596338
	<chem>Cc1ccc(O)c(C(=O)NCC(C)CNC(=O)c2ccncc2)cn1</chem>	ENAMINE PV-003300703421
	<chem>Cc1cc(O)nc(C(=O)N2CC(CCN2C)c1</chem>	ENAMINE Z2212459631

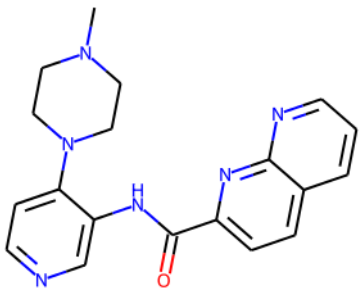
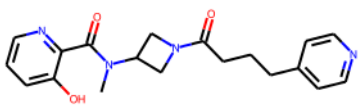
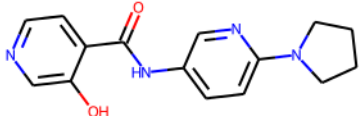
Chemical Structure	SMILES	Vendor
	<chem>Oc1cncc1-c1nc(-c2cncc(F)c2)nn1Cc1ccncc1</chem>	ENAMINE PV-003589856981
	<chem>CC(=O)N(c1ccc(NC(=O)c2ccccc2O)cc1)C1CC1</chem>	ENAMINE Z2232437036
	<chem>Nc1ncc2c(n1)CN(Cc1nncc(N3CCCCC3)o1)C2</chem>	ENAMINE Z4275407035

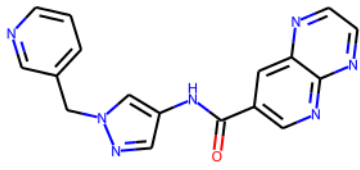
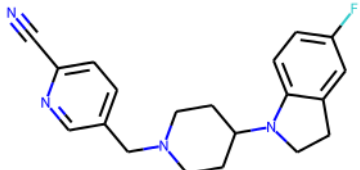
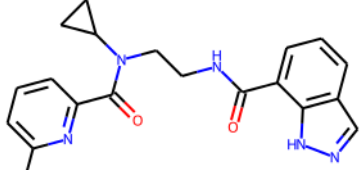
Chemical Structure	SMILES	Vendor
	<chem>CN(CCCN(C)C(=O)c1cc2ncccc2[nH]1)C(=O)Cc1cn[nH]c1</chem>	ENAMINE PV-002774371686
	<chem>Cc1cccc(N(C)C(=O)c2cnc(C(=O)N3CCCC3)n2)n1</chem>	ENAMINE Z1261297794
	<chem>O=C(NCc1ccnc(-c2ccccn2)n1)c1ccn2cnnc2c1</chem>	ENAMINE PV-003036501924

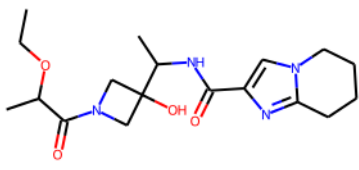
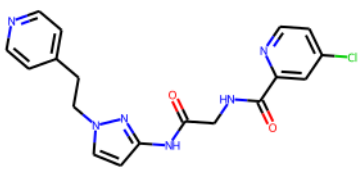
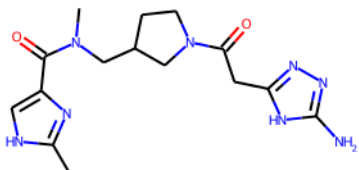
Chemical Structure	SMILES	Vendor
	<chem>COC(=O)c1ccc(C(=O)N[C@@H](Cc2cn(C)cn2)C(=O)O)cn1</chem>	ENAMINE PV-002940074911
	<chem>CN(C)c1nn(C)cc1-c1noc(-c2cccc3nn(C)cc23)n1</chem>	ENAMINE Z4564247284
	<chem>CC(CNC(=O)c1ccc(O)c(N)n1)N(C)C(=O)CCc1ccncc1</chem>	ENAMINE PV-003833522780

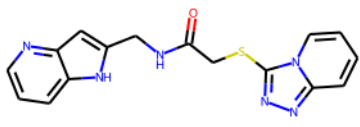
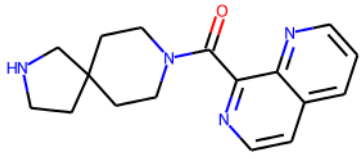
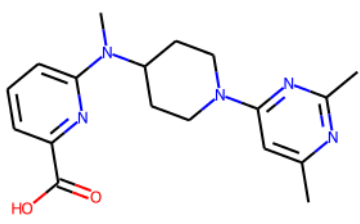
Chemical Structure	SMILES	Vendor
	<chem>O=C(CNC(=O)c1cccn1)Nc1ccc(C(=O)Nc2cccn2)cc1</chem>	ENAMINE Z1333654288
	<chem>CC(CNC(=O)c1ccn2nccc2n1)c1ccncc1</chem>	ENAMINE PV-002346920733
	<chem>O=C(Nc1cn2cccnc2n1)c1cc2ccncc2c(O)n1</chem>	ENAMINE PV-003664638788

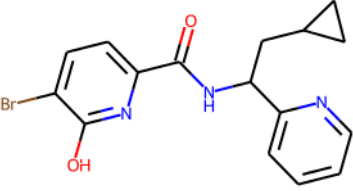
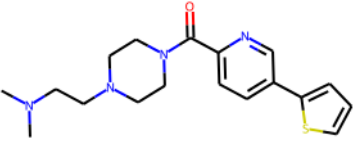
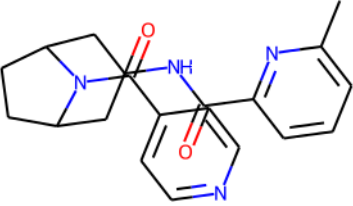
Chemical Structure	SMILES	Vendor
	<chem>CC1CN(C)CCN1C(=O)c1c</chem> <chem>cc(C(=O)O)nc1O</chem>	ENAMINE PV-003234061552
	<chem>Cc1nc(-c2nc3cncnc3nc</chem> <chem>2O)n(Cc2ccnc2)n1</chem>	ENAMINE PV-003736214891
	<chem>COc1cc(C)nc(Sc2nnc(-</chem> <chem>c3cncn3)n2C)n1</chem>	ENAMINE Z1439515070

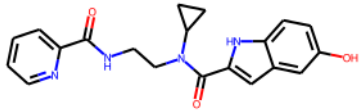
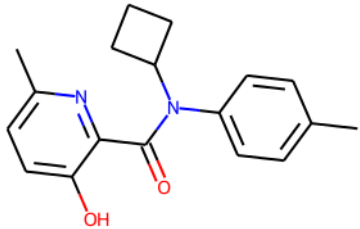
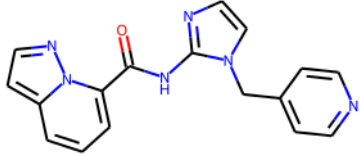
Chemical Structure	SMILES	Vendor
	<chem>CN1CCN(c2ccncc2NC(=O)c2ccc3cccn3n2)CC1</chem>	ENAMINE Z2623854964
	<chem>CN(C(=O)c1ncccc1O)C1CN(C(=O)CCCC2CCNCC2)C1</chem>	ENAMINE PV-003496622986
	<chem>O=C(Nc1ccc(N2CCCC2)nc1)c1ccncc1O</chem>	ENAMINE Z1373385559

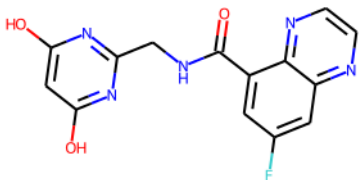
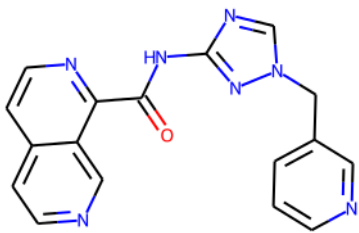
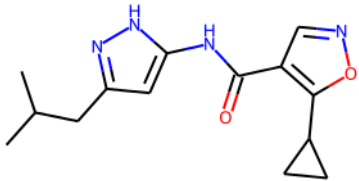
Chemical Structure	SMILES	Vendor
	<chem>O=C(Nc1cnn(Cc2ccnc2)c1)c1cnc2nccnc2c1</chem>	ENAMINE Z1675628706
	<chem>N#Cc1ccc(CN2CCC(N3CCc4cc(F)ccc43)CC2)cn1</chem>	ENAMINE Z3515334684
	<chem>Cc1cccc(C(=O)N(CCNC(=O)c2cccc3cn[nH]c23)C2CC2)n1</chem>	ENAMINE PV-001464861322

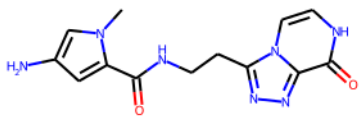
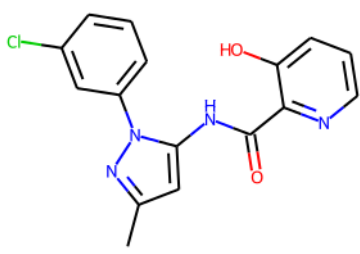
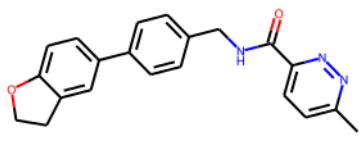
Chemical Structure	SMILES	Vendor
	<chem>CCOC(C)C(=O)N1CC(O)(C(C)NC(=O)c2cn3c(n2)CCCC3)C1</chem>	ENAMINE PV-004005824038
	<chem>O=C(CNC(=O)c1cc(Cl)cnc1)Nc1ccn(CCc2ccncc2)n1</chem>	ENAMINE Z984446284
	<chem>Cc1nc(C(=O)N(C)CC2CCN(C(=O)Cc3nnc(N)[nH]3)C2)c[nH]1</chem>	ENAMINE PV-003584918101

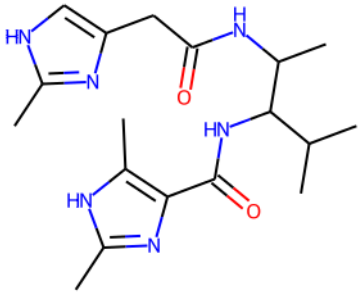
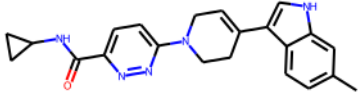
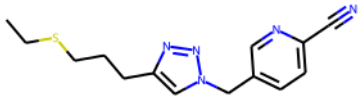
Chemical Structure	SMILES	Vendor
	<chem>O=C(CSc1nnc2ccccc12)NCc1cc2ncccc2[nH]1</chem>	ENAMINE PV-002709273654
	<chem>O=C(c1nccc2cccnc12)N1CCC2(CCNC2)CC1</chem>	ENAMINE Z3104794088
	<chem>Cc1cc(N2CCC(N(C)c3cc(C)cc(C(=O)O)n3)CC2)nc(C)n1</chem>	ENAMINE Z2358630674

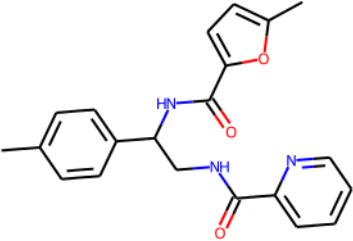
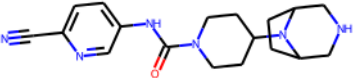
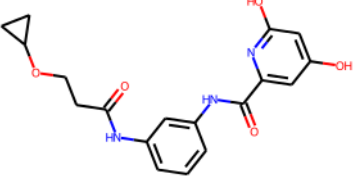
Chemical Structure	SMILES	Vendor
	<chem>O=C(NC(CC1CC1)c1ccccn1)c1ccc(Br)c(O)n1</chem>	ENAMINE PV-003961765830
	<chem>CN(C)CCN1CCN(C(=O)c2ccc(-c3cccs3)cn2)CC1</chem>	ENAMINE Z4348130665
	<chem>Cc1cccc(C(=O)NC2CC3C CC(C2)N3C(=O)c2ccncc2)n1</chem>	ENAMINE Z3726135997

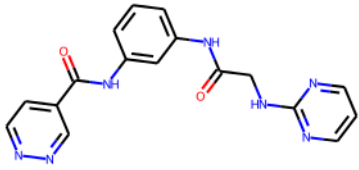
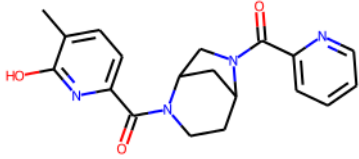
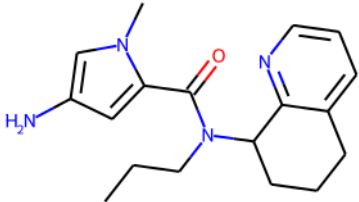
Chemical Structure	SMILES	Vendor
	<chem>O=C(NCCN(C(=O)c1cc2c c(O)ccc2[nH]1)C1CC1)c1cccn1</chem>	ENAMINE PV-003980459953
	<chem>Cc1ccc(N(C(=O)c2nc(C)ccc2O)C2CCC2)cc1</chem>	ENAMINE PV-003889617014
	<chem>O=C(Nc1nccn1Cc1cncc 1)c1cccc2ccnn12</chem>	ENAMINE PV-003663788839

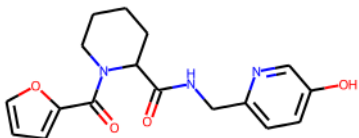
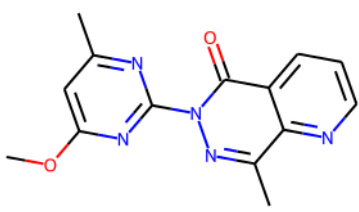
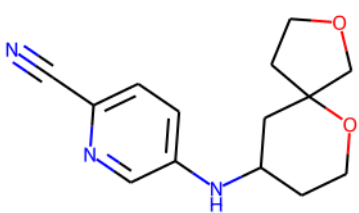
Chemical Structure	SMILES	Vendor
	<chem>O=C(NCc1nc(O)cc(O)n1)c1cc(F)cc2nccnc12</chem>	ENAMINE PV-002292012664
	<chem>O=C(Nc1ncn(Cc2ccccc2)n1)c1ncccc2ccncc12</chem>	ENAMINE PV-003421043056
	<chem>CC(C)Cc1cc(NC(=O)c2c[nH]n2)c[nH]1</chem>	ENAMINE Z1750162351

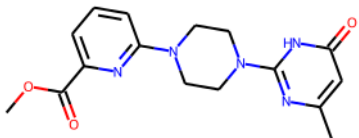
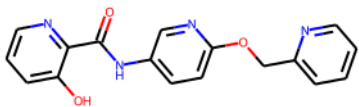
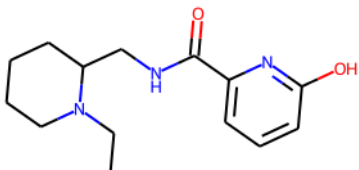
Chemical Structure	SMILES	Vendor
	<chem>Cc1cc(N)cc1C(=O)NCCc1nnc2c(=O)[nH]ccn12</chem>	ENAMINE PV-003068919678
	<chem>Cc1cc(NC(=O)c2ncccc2O)n(-c2cccc(Cl)c2)n1</chem>	ENAMINE Z1746395485
	<chem>Cc1ccc(C(=O)NCc2ccc(-c3ccc4c(c3)CCO4)cc2)nn1</chem>	ENAMINE PV-002535483222

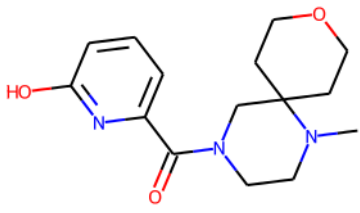
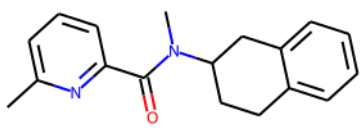
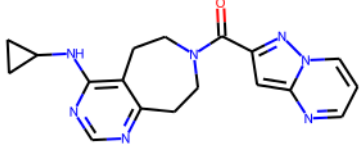
Chemical Structure	SMILES	Vendor
	<chem>Cc1nc(CC(=O)NC(C)C(NC(=O)c2nc(C)[nH]c2C)C(C)C)c[nH]1</chem>	ENAMINE PV-004050219354
	<chem>Cc1ccc2c(C3=CCN(c4cc(C(=O)NC5CC5)nn4)CC3)c[nH]c2c1</chem>	ENAMINE Z1815595691
	<chem>CCSCCCc1cn(Cc2ccc(C#N)nc2)nn1</chem>	ENAMINE Z4025533373

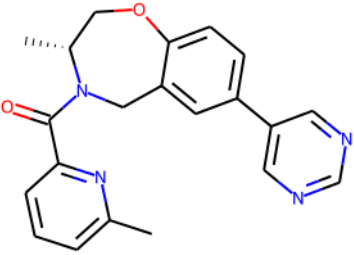
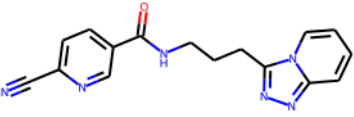
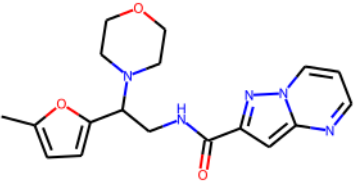
Chemical Structure	SMILES	Vendor
	<chem>Cc1ccc(C(CNC(=O)c2cccn2)NC(=O)c2ccc(C)o2)cc1</chem>	ENAMINE PV-003967563864
	<chem>N#Cc1ccc(NC(=O)N2CCC(N3C4CCC3CNC4)CC2)cn1</chem>	ENAMINE Z2927515383
	<chem>O=C(CCOC1CC1)Nc1cccc(NC(=O)c2cc(O)cc(O)n2)c1</chem>	ENAMINE PV-003129864012

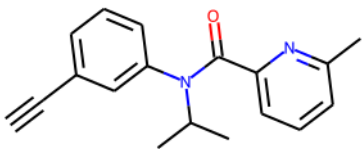
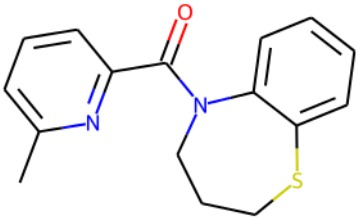
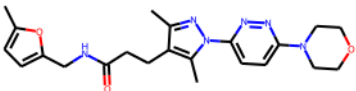
Chemical Structure	SMILES	Vendor
	<chem>O=C(CNc1ncccn1)Nc1ccc(NC(=O)c2ccnnc2)c1</chem>	ENAMINE PV-003567673554
	<chem>Cc1ccc(C(=O)N2CCC3CC2CN3C(=O)c2ccccn2)nc1O</chem>	ENAMINE PV-003621008989
	<chem>CCCN(C(=O)c1cc(N)cn1)C1CCCCc2ccnnc21</chem>	ENAMINE Z4207017952

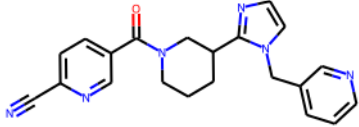
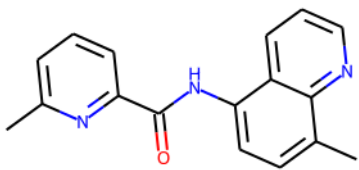
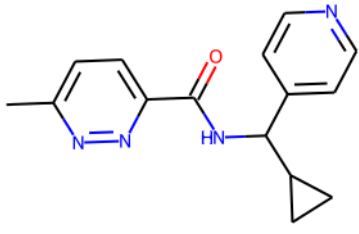
Chemical Structure	SMILES	Vendor
	<chem>O=C(NCc1ccc(O)cn1)C1CCCCN1C(=O)c1ccco1</chem>	ENAMINE Z4218925553
	<chem>COc1cc(C)nc(-n2nc(C)c3ncccc3c2=O)n1</chem>	ENAMINE PV-002922250337
	<chem>N#Cc1ccc(NC2CCOC3(CCOC3)C2)cn1</chem>	ENAMINE Z1577080799

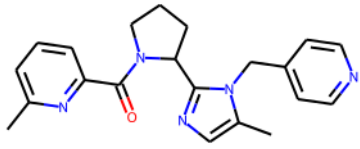
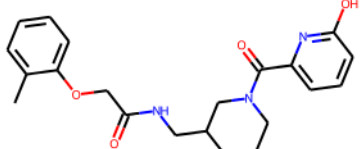
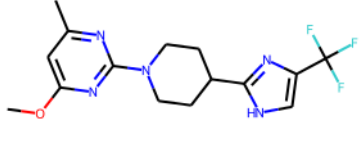
Chemical Structure	SMILES	Vendor
	<chem>COC(=O)c1cccc(N2CCN(c3nc(C)cc(=O)[nH]3)CC2)n1</chem>	ENAMINE Z2861690732
	<chem>O=C(Nc1ccc(OCc2cccn2)nc1)c1ncccc1O</chem>	ENAMINE PV-002717285255
	<chem>CCN1CCCCC1CNC(=O)c1cccc(O)n1</chem>	MCULE MCULE-8428478358

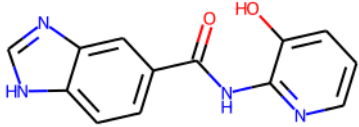
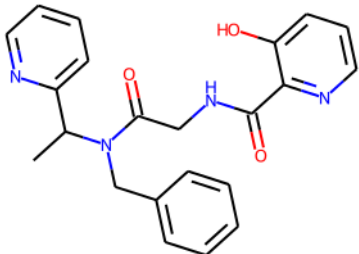
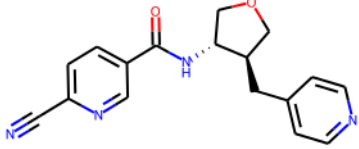
Chemical Structure	SMILES	Vendor
	<chem>CN1CCN(C(=O)c2cccc(O)n2)CC12CCOCC2</chem>	MCULE MCULE-7228537800
	<chem>Cc1cccc(C(=O)N(C)C2Cc3ccccc3C2)n1</chem>	MCULE MCULE-1313181678
	<chem>O=C(c1cc2ncccn2n1)N1CCc2ncnc(NC3CC3)c2CC1</chem>	MCULE MCULE-1171876743

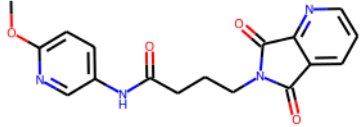
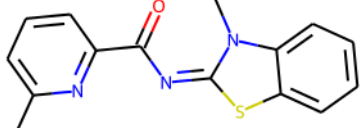
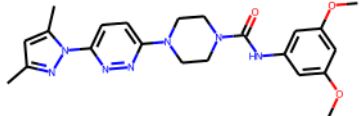
Chemical Structure	SMILES	Vendor
	<chem>Cc1cccc(C(=O)N2Cc3cc(-c4cnnc4)ccc3OC[C@H]2C)n1</chem>	MCULE MCULE-3927951385
	<chem>N#Cc1ccc(C(=O)NCCCc2nnc3ccccn23)cn1</chem>	MCULE MCULE-2783374498
	<chem>Cc1ccc(C(CNC(=O)c2cc3ncccn3n2)N2CCOCC2)o1</chem>	MCULE MCULE-5963365200

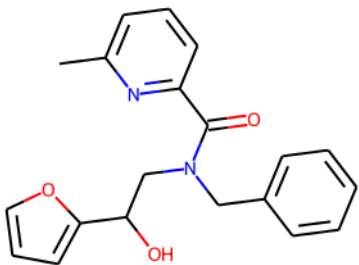
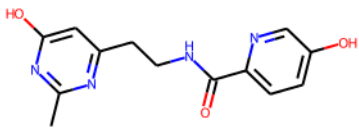
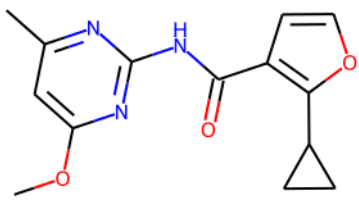
Chemical Structure	SMILES	Vendor
	<chem>C#Cc1ccc(N(C(=O)c2cc(C)cn2)C(C)C)c1</chem>	MCULE MCULE-5872044089
	<chem>Cc1ccc(C(=O)N2CCCSccc2n1)</chem>	MCULE MCULE-9117364590
	<chem>Cc1ccc(CNC(=O)CCc2c(C)nn(-c3ccc(N4CCOCC4)nn3)c2C)o1</chem>	MCULE MCULE-8840129925

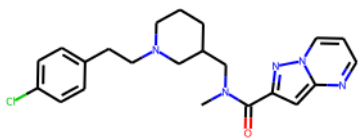
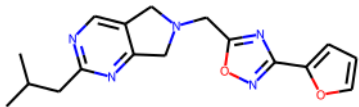
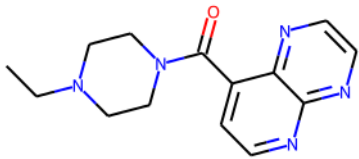
Chemical Structure	SMILES	Vendor
	<chem>N#Cc1ccc(C(=O)N2CCCC(c3nccn3Cc3ccnc3)C2)cn1</chem>	MCULE MCULE-6001835840
	<chem>Cc1cccc(C(=O)Nc2ccc(C)c3ncccc23)n1</chem>	MCULE MCULE-1312161684
	<chem>Cc1ccc(C(=O)NC(c2ccncc2)C2CC2)nn1</chem>	MCULE MCULE-5428575173

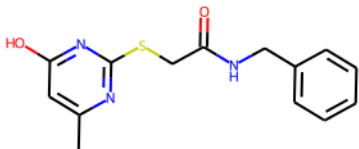
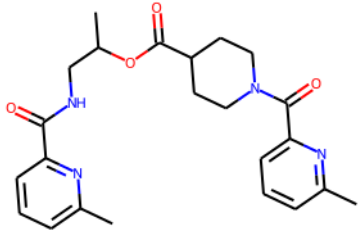
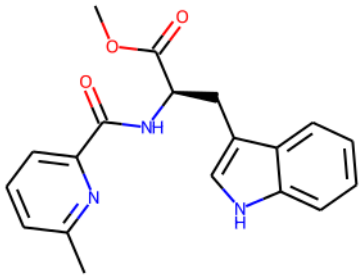
Chemical Structure	SMILES	Vendor
	<chem>Cc1ccc(C(=O)N2CCCC2c2ncc(C)n2Cc2ccncc2)n1</chem>	MCULE MCULE-1702329592
	<chem>Cc1ccc(OCC(=O)NCC1CCCC1C(=O)c2ccc(O)n2)C1</chem>	MCULE MCULE-8410248586
	<chem>COc1cc(C)nc(N2CCCC2c3nc(C(F)(F)F)c[nH]3)CC2)n1</chem>	MCULE MCULE-8249697523

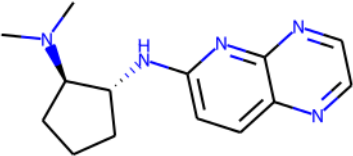
Chemical Structure	SMILES	Vendor
	<chem>O=C(Nc1ncccc1O)c1ccc2[nH]cnc2c1</chem>	MCULE MCULE-1297202557
	<chem>CC(c1ccccn1)N(Cc1ccc1)C(=O)CNC(=O)c1ncccc1O</chem>	MCULE MCULE-1872430624
	<chem>N#Cc1ccc(C(=O)N[C@@H](COCCc2ccncc2)cn1</chem>	MCULE MCULE-9309105329

Chemical Structure	SMILES	Vendor
	<chem>COc1ccc(NC(=O)CCCN2C(=O)c3ccncc3C2=O)cn1</chem>	MCULE MCULE-9076629149
	<chem>Cc1cccc(C(=O)N=c2sc3ccccc3n2C)n1</chem>	MCULE MCULE-2849820140
	<chem>COc1cc(NC(=O)N2CCN(c3ccc(-n4nc(C)cc4C)nn3)CC2)cc(OC)c1</chem>	MCULE MCULE-5060133512

Chemical Structure	SMILES	Vendor
	<chem>Cc1cccc(C(=O)N(Cc2ccccc2)CC(O)c2ccco2)n1</chem>	MCULE MCULE-6816850428
	<chem>Cc1nc(O)cc(CCNC(=O)c2ccc(O)cn2)n1</chem>	MCULE MCULE-6013078434
	<chem>COc1cc(C)nc(NC(=O)c2ccoc2C3CC3)n1</chem>	MCULE MCULE-3482072072

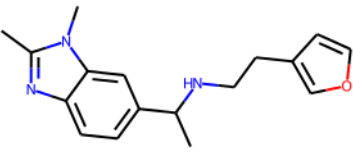
Chemical Structure	SMILES	Vendor
	<chem>CN(CC1CCCN(CCc2ccc(Cl)cc2)C1)C(=O)c1cc2ncccn2n1</chem>	MCULE MCULE-7071715560
	<chem>CC(C)Cc1ncc2c(n1)CN(Cc1nc(-c3ccco3)no1)C2</chem>	MCULE MCULE-8855197724
	<chem>CCN1CCN(C(=O)c2ccnc3nccnc23)CC1</chem>	MCULE MCULE-9852875024

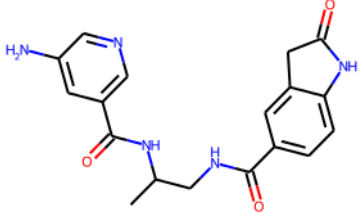
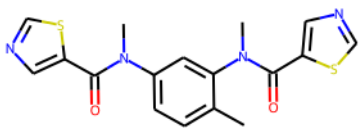
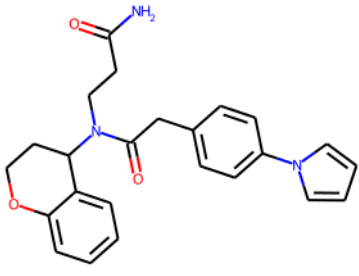
Chemical Structure	SMILES	Vendor
	<chem>Cc1cc(O)nc(SCC(=O)NCc2ccccc2)n1</chem>	MCULE MCULE-8428224146
	<chem>Cc1cccc(C(=O)NCC(C)OC(=O)C2CCN(C(=O)c3cc cc(C)n3)CC2)n1</chem>	MCULE MCULE-9036671008
	<chem>COC(=O)[C@@H](Cc1c[nH]c2ccccc12)NC(=O)c1cccc(C)n1</chem>	MCULE MCULE-2903378343

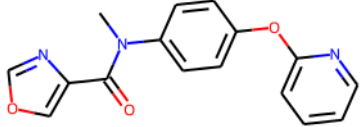
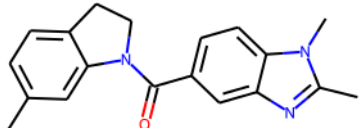
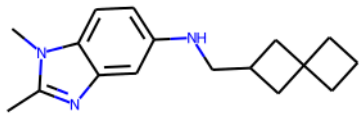
Chemical Structure	SMILES	Vendor
	<chem>CN(C)[C@@H]1CCCC[C@H]1Nc1ccc2ncnc2n1</chem>	MCULE MCULE-4092218565

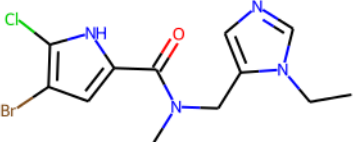
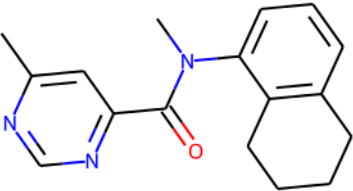
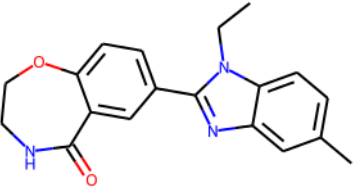
2 MID1

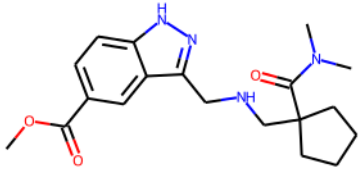
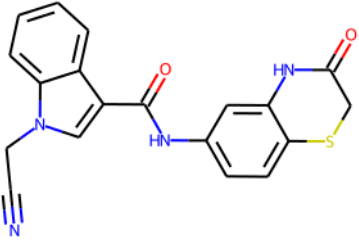
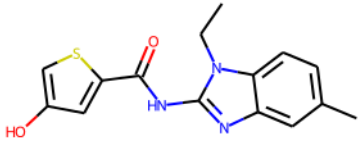
UniProtKB entry O15344

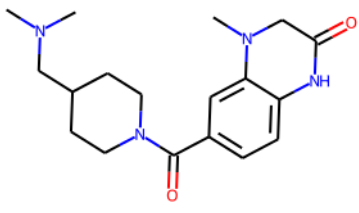
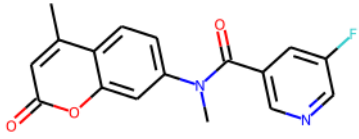
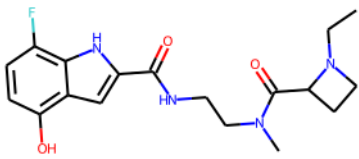
Chemical Structure	SMILES	Vendor
	<chem>Cc1nc2ccc(C(C)NCCc3ccoc3)cc2n1C</chem>	ENAMINE Z4043091867

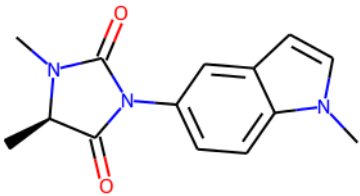
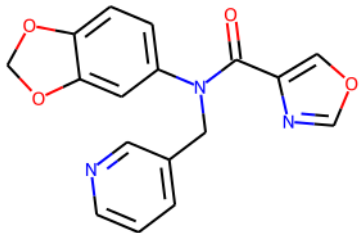
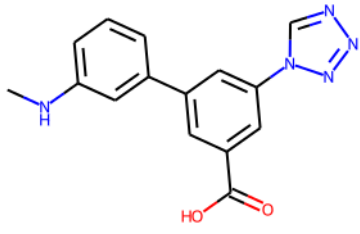
Chemical Structure	SMILES	Vendor
	<chem>CC(CNC(=O)c1ccc2c(c1)CC(=O)N2)NC(=O)c1cncc(N)c1</chem>	ENAMINE PV-002743978711
	<chem>Cc1ccc(N(C)C(=O)c2cnsc2)cc1N(C)C(=O)c1cnsc1</chem>	ENAMINE Z1458964392
	<chem>NC(=O)CCN(C(=O)Cc1ccc(-n2cccc2)cc1)C1CCOc2ccccc21</chem>	ENAMINE Z3277690545

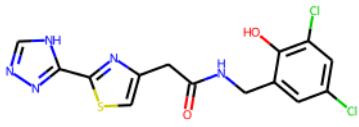
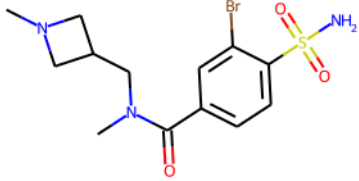
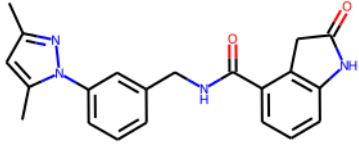
Chemical Structure	SMILES	Vendor
	<chem>CN(C(=O)c1cncn1)c1ccc(Oc2ccccc2)cc1</chem>	ENAMINE Z1210248944
	<chem>Cc1ccc2c(c1)N(C(=O)c1ccc2c1)nc(C)n3C)CC2</chem>	ENAMINE Z969087856
	<chem>Cc1nc2cc(NCC3CC4(CCC4)C3)ccc2n1C</chem>	ENAMINE PV-003008994626

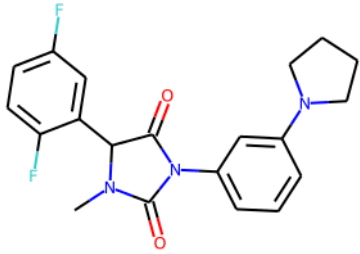
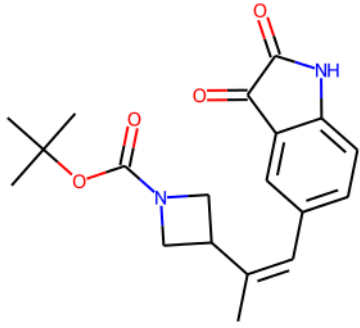
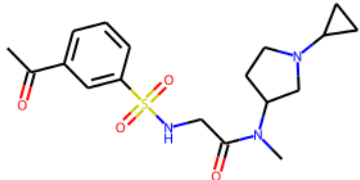
Chemical Structure	SMILES	Vendor
	<chem>CCn1cncc1CN(C)C(=O)c1cc(Br)c(Cl)[nH]1</chem>	ENAMINE Z3612430213
	<chem>Cc1cc(C(=O)N(C)c2ccc3c2CCCC3)ncn1</chem>	ENAMINE Z4471855420
	<chem>CCn1c(-c2ccc3c(c2)C(=O)NCCO3)nc2cc(C)ccc21</chem>	ENAMINE PV-002871464366

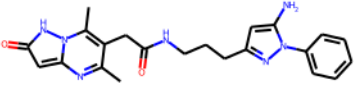
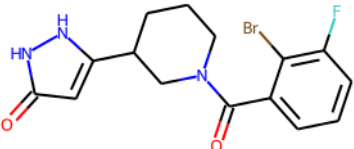
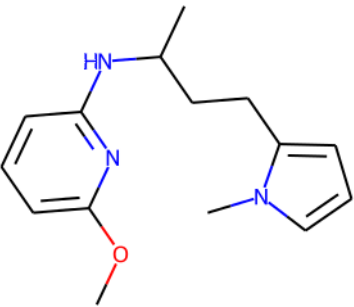
Chemical Structure	SMILES	Vendor
	<chem>COC(=O)c1ccc2[nH]nc(CNCC3(C(=O)N(C)C)CCCC3)c2c1</chem>	ENAMINE Z4195189592
	<chem>N#CCn1cc(C(=O)Nc2ccc3c(c2)NC(=O)CS3)c2cccc21</chem>	ENAMINE Z803696656
	<chem>CCn1c(NC(=O)c2cc(O)cs2)nc2cc(C)ccc21</chem>	ENAMINE Z1600619017

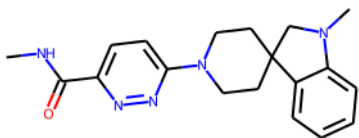
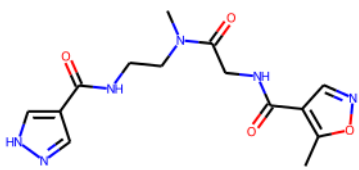
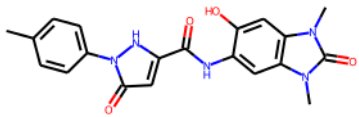
Chemical Structure	SMILES	Vendor
	<chem>CN(C)CC1CCN(C(=O)c2ccc3c(c2)N(C)CC(=O)N3)CC1</chem>	ENAMINE Z4639053086
	<chem>Cc1cc(=O)oc2cc(N(C)C(=O)c3cncc(F)c3)ccc12</chem>	ENAMINE Z2099958890
	<chem>CCN1CCC1C(=O)N(C)CCN(C(=O)c1cc2c(O)ccc(F)c2[nH]1)</chem>	ENAMINE PV-004075672981

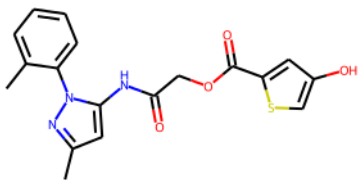
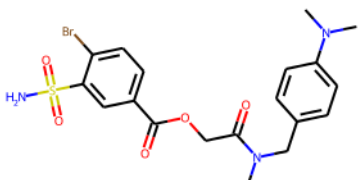
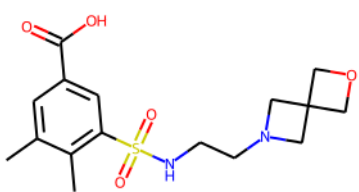
Chemical Structure	SMILES	Vendor
	<chem>C[C@@H]1C(=O)N(c2ccc3c(ccn3C)c2)C(=O)N1C</chem>	ENAMINE Z3499889660
	<chem>O=C(c1cocc1)N(Cc1cccnc1)c1ccc2c(c1)OCO2</chem>	ENAMINE PV-003089972107
	<chem>CNc1cccc(-c2cc(C(=O)O)cc(-n3cnnn3)c2)c1</chem>	ENAMINE PV-002863981953

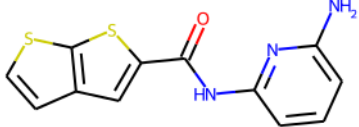
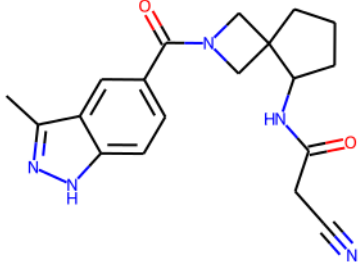
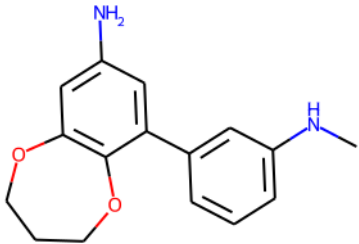
Chemical Structure	SMILES	Vendor
	<chem>O=C(Cc1csc(-c2nnc[nH]2)n1)NCc1cc(Cl)cc(Cl)c1O</chem>	ENAMINE Z2140876372
	<chem>CN1CC(CN(C)C(=O)c2cc(S(N)(=O)=O)c(Br)c2)C1</chem>	ENAMINE Z2645164621
	<chem>Cc1cc(C)n(-c2cccc(CN(C(=O)c3cccc4c3CC(=O)N4)c2)n1</chem>	ENAMINE PV-003963826253

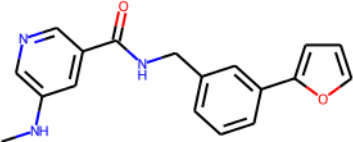
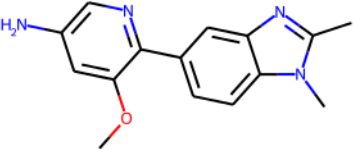
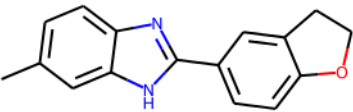
Chemical Structure	SMILES	Vendor
	<chem>CN1C(=O)N(c2cccc(N3CCCC3)c2)C(=O)C1c1cc(F)ccc1F</chem>	ENAMINE Z1891896658
	<chem>CC(=Cc1ccc2c(c1)C(=O)C(=O)N2)C1CN(C(=O)OC(C)(C)C)C1</chem>	ENAMINE Z4122021775
	<chem>CC(=O)c1cccc(S(=O)(=O)NCC(=O)N(C)C2CCN(C3CC3)C2)c1</chem>	ENAMINE Z2173975721

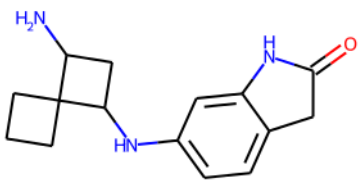
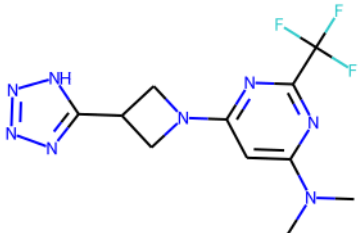
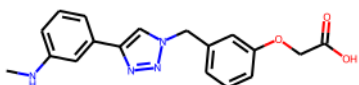
Chemical Structure	SMILES	Vendor
	<chem>Cc1nc2cc(=O)[nH]n2c(C)c1CC(=O)NCCCCc1cc(N)n(-c2ccccc2)n1</chem>	ENAMINE Z1130909537
	<chem>O=C(c1cccc(F)c1Br)N1CCCCC1C(=O)c2ccccc2</chem>	ENAMINE Z4238154412
	<chem>COc1cccc(NC(C)CCc2cccn2C)n1</chem>	ENAMINE Z2492044141

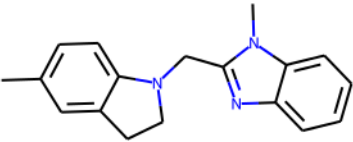
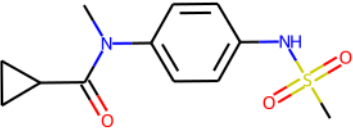
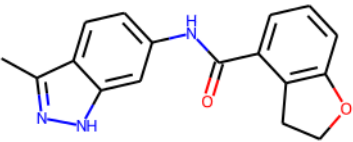
Chemical Structure	SMILES	Vendor
	<chem>CNC(=O)c1ccc(N2CCC3(CC2)CN(C)c2ccccc23)nn1</chem>	ENAMINE Z3833651577
	<chem>Cc1oncc1C(=O)NCC(=O)N(C)CCNC(=O)c1cn[nH]c1</chem>	ENAMINE PV-003265830747
	<chem>Cc1ccc(-n2[nH]c(C(=O)Nc3cc4c(cc3O)n(C)c(=O)n4C)cc2=O)cc1</chem>	ENAMINE Z2206119445

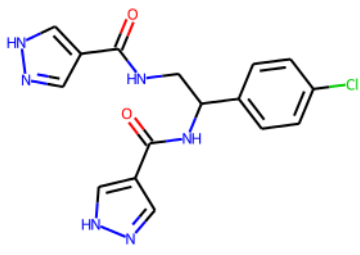
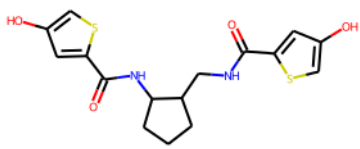
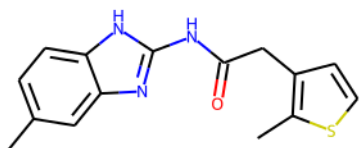
Chemical Structure	SMILES	Vendor
	<chem>Cc1cc(NC(=O)COC(=O)c2cc(O)cs2)n(-c2ccccc2C)n1</chem>	ENAMINE Z1179750400
	<chem>CN(Cc1ccc(N(C)C)cc1)C(=O)COC(=O)c1ccc(Br)cc1</chem>	ENAMINE Z418173410
	<chem>Cc1cc(C(=O)O)cc(S(=O)(=O)NCCN2CC3(COC3)C2)c1C</chem>	ENAMINE Z3569486555

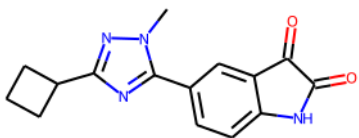
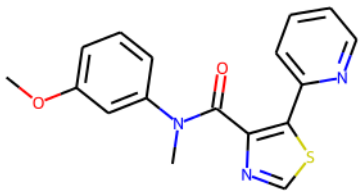
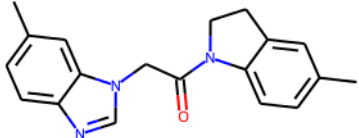
Chemical Structure	SMILES	Vendor
	<chem>Nc1cccc(NC(=O)c2cc3ccsc3s2)n1</chem>	ENAMINE PV-002793845864
	<chem>Cc1n[nH]c2ccc(C(=O)N3CC4(CCCC4NC(=O)CC#N)C3)cc12</chem>	ENAMINE PV-003098541473
	<chem>CNc1cccc(-c2cc(N)cc3c2OCCCO3)c1</chem>	ENAMINE Z3347312779

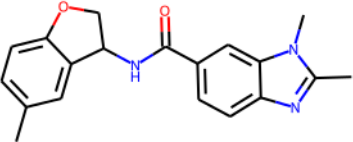
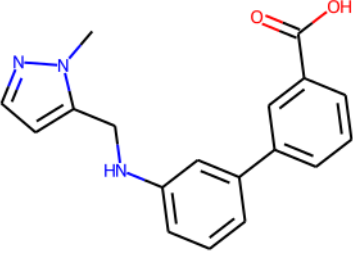
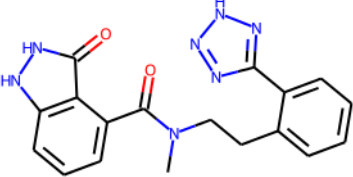
Chemical Structure	SMILES	Vendor
	<chem>CNc1cncc(C(=O)NCc2ccc(-c3ccco3)c2)c1</chem>	ENAMINE PV-003145902185
	<chem>COc1cc(N)cnc1-c1ccc2c(c1)nc(C)n2C</chem>	ENAMINE PV-002873537581
	<chem>Cc1ccc2nc(-c3ccc4c(c3)CCO4)[nH]c2c1</chem>	ENAMINE Z1527368608

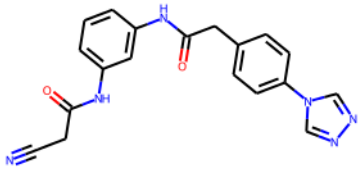
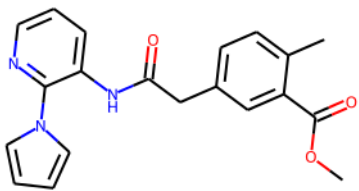
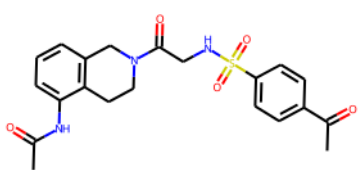
Chemical Structure	SMILES	Vendor
	<chem>NC1CC(Nc2ccc3c(c2)NC(=O)C3)C12CCC2</chem>	ENAMINE Z2927004863
	<chem>CN(C)c1cc(N2CC(c3nnn[nH]3)C2)nc(C(F)(F)F)n1</chem>	ENAMINE Z4231022943
	<chem>CNc1cccc(-c2cn(Cc3ccc(OCC(=O)O)c3)nn2)c1</chem>	ENAMINE PV-002918771940

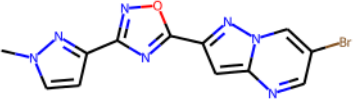
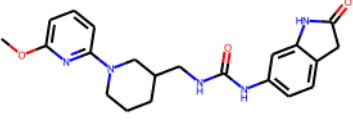
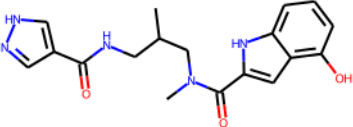
Chemical Structure	SMILES	Vendor
	<chem>Cc1ccc2c(c1)CCN2Cc1nc2ccccc2n1C</chem>	ENAMINE Z1584264527
	<chem>CN(C(=O)C1CC1)c1ccc(NS(C)(=O)=O)cc1</chem>	ENAMINE Z2897397642
	<chem>Cc1n[nH]c2cc(NC(=O)c3ccccc3OCO4)ccc12</chem>	ENAMINE PV-003237725727

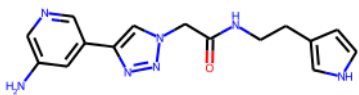
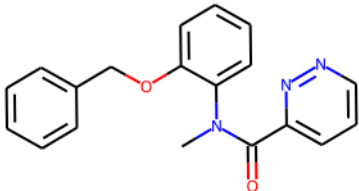
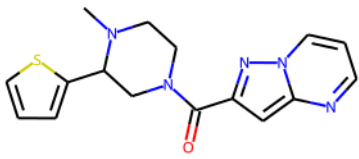
Chemical Structure	SMILES	Vendor
	<chem>O=C(NCC(NC(=O)c1cn[nH]c1)c1ccc(Cl)cc1)c1cn[nH]c1</chem>	ENAMINE Z1997613277
	<chem>O=C(NCC1CCCC1NC(=O)c1cc(O)cs1)c1cc(O)cs1</chem>	ENAMINE Z2631523968
	<chem>Cc1ccc2[nH]c(NC(=O)CCc3ccsc3)nc2c1</chem>	ENAMINE Z2229661170

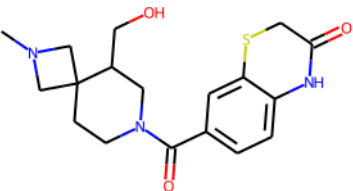
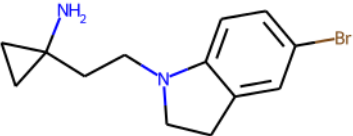
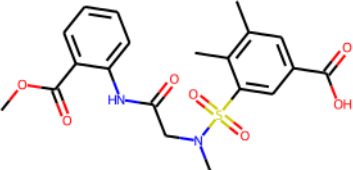
Chemical Structure	SMILES	Vendor
	<chem>Cn1nc(C2CCC2)nc1-c1ccc2c(c1)C(=O)C(=O)N2</chem>	ENAMINE Z3506156186
	<chem>COc1ccc(N(C)C(=O)c2ncsc2-c2cccn2)c1</chem>	ENAMINE PV-003425953794
	<chem>Cc1ccc2c(c1)CCN2C(=O)Cn1cnc2ccc(C)cc21</chem>	ENAMINE Z1952693217

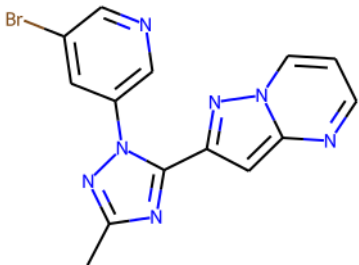
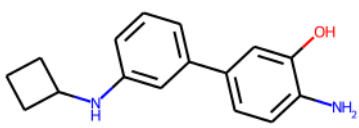
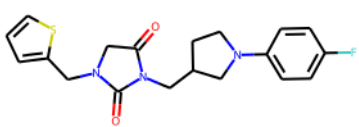
Chemical Structure	SMILES	Vendor
	<chem>Cc1ccc2c(c1)C(NC(=O)c1ccc3nc(C)n(C)c3c1)CO2</chem>	ENAMINE Z1952486906
	<chem>Cn1cccc1CNc1cccc(-c2cccc(C(=O)O)c2)c1</chem>	ENAMINE PV-002883746856
	<chem>CN(CCc1cccc1-c1nn[nH]n1)C(=O)c1cccc2[nH][nH]c(=O)c12</chem>	ENAMINE PV-004126289087

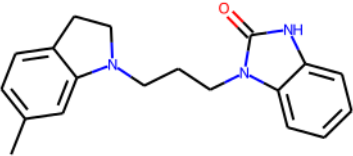
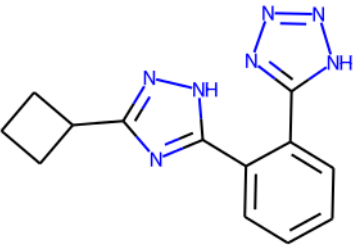
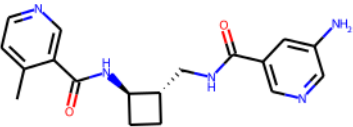
Chemical Structure	SMILES	Vendor
	<chem>N#CCCC(=O)Nc1cccc(NC(=O)Cc2ccc(-n3cnnc3)cc2)c1</chem>	ENAMINE PV-003993095261
	<chem>COC(=O)c1cc(CC(=O)Nc2cccnc2-n2ccccc2)ccc1C</chem>	ENAMINE PV-003765651242
	<chem>CC(=O)Nc1cccc2c1CCN(C(=O)CNS(=O)(=O)c1ccc(C(=O)O)cc1)C2</chem>	ENAMINE Z758532824

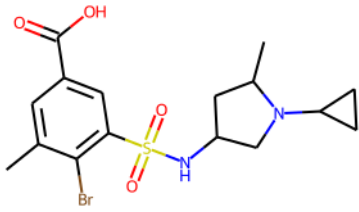
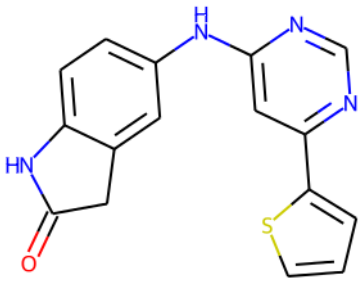
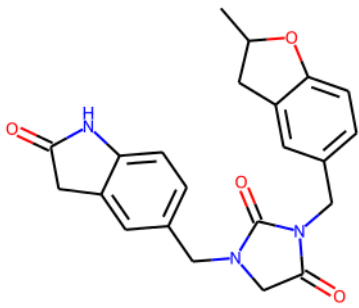
Chemical Structure	SMILES	Vendor
	<chem>Cn1ccc(-c2noc(-c3cc4ncc(Br)cn4n3)n2)n1</chem>	ENAMINE PV-003035459961
	<chem>COc1ccc(N2CCCC(CNC(=O)Nc3ccc4c(c3)NC(=O)C4)C2)n1</chem>	ENAMINE Z4466407245
	<chem>CC(CNC(=O)c1cn[nH]c1)CN(C)C(=O)c1cc2c(O)cccc2[nH]1</chem>	ENAMINE PV-003126568411

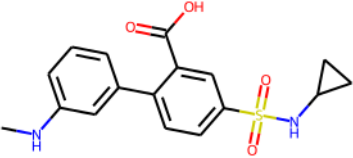
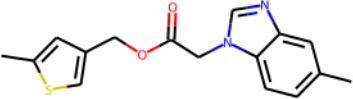
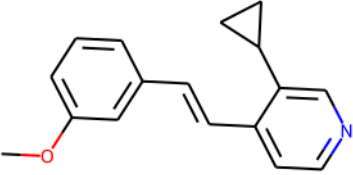
Chemical Structure	SMILES	Vendor
	<chem>Nc1cncc(-c2cn(CC(=O)NCCc3cc[nH]c3)nn2)c1</chem>	ENAMINE PV-002804674257
	<chem>CN(C(=O)c1cccnn1)c1c cccc1OCc1ccccc1</chem>	ENAMINE PV-002128074355
	<chem>CN1CCN(C(=O)c2cc3ncc cn3n2)CC1c1cccs1</chem>	ENAMINE Z4472169220

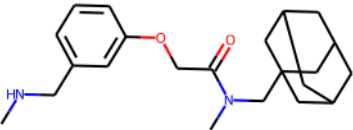
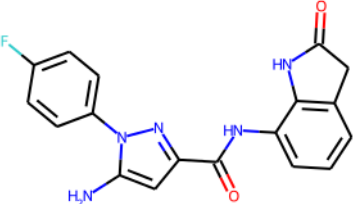
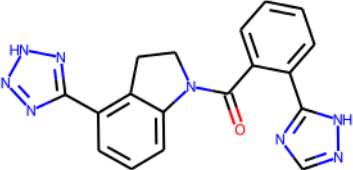
Chemical Structure	SMILES	Vendor
	<chem>CN1CC2(CCN(C(=O)c3cc</chem> <chem>c4c(c3)SCC'(=O)N4)CC2CO)C1</chem>	ENAMINE Z3898848431
	<chem>NC1(CCN2CCc3cc(Br)ccc32)CC1</chem>	ENAMINE PV-003620578880
	<chem>COC(=O)c1ccccc1NC(=O</chem> <chem>)CN(C)S(=O)(=O)c1cc(</chem> <chem>C(=O)O)cc(C)c1C</chem>	ENAMINE Z240302414

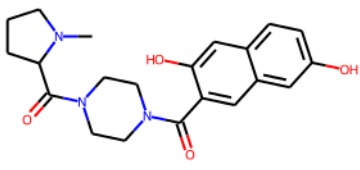
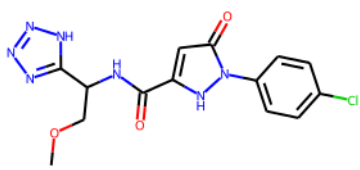
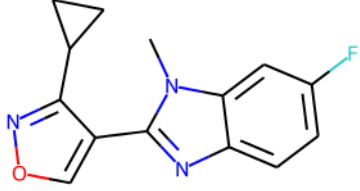
Chemical Structure	SMILES	Vendor
	<chem>Cc1nc(-c2cc3ncccn3n2)n(-c2cncc(Br)c2)n1</chem>	ENAMINE PV-003521801081
	<chem>Nc1ccc(-c2cccc(NC3CCCC3)c2)cc1O</chem>	ENAMINE Z3347767893
	<chem>O=C1CN(Cc2cccs2)C(=O)N1CC1CCN(c2ccc(F)cc2)C1</chem>	ENAMINE Z3878214016

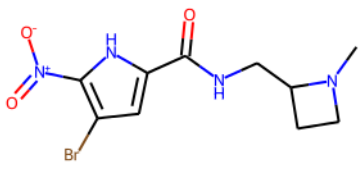
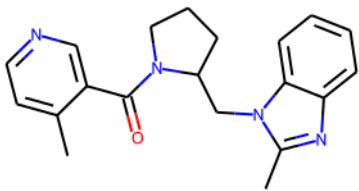
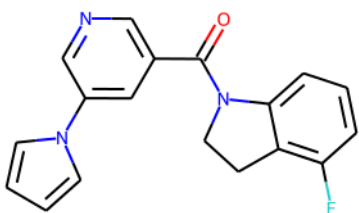
Chemical Structure	SMILES	Vendor
	<chem>Cc1ccc2c(c1)N(CCCn1c(=O)[nH]c3ccccc31)CC2</chem>	ENAMINE PV-002396477500
	<chem>c1ccc(-c2nc(C3CCCC3)n[nH]2)c(-c2nnn[nH]2)c1</chem>	ENAMINE Z4079370393
	<chem>Cc1ccncc1C(=O)N[C@@H]1CC[C@H]1CNC(=O)c1cncc(N)c1</chem>	ENAMINE PV-003546210169

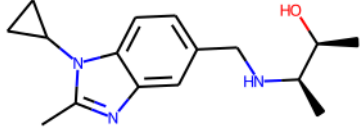
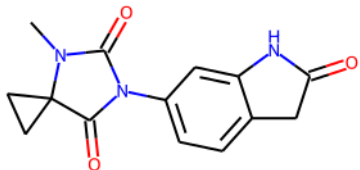
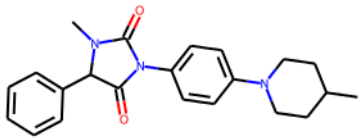
Chemical Structure	SMILES	Vendor
	<chem>Cc1cc(C(=O)O)cc(S(=O)(=O)NC2CC(C)N(C3CC3)C2)c1Br</chem>	ENAMINE Z1682268691
	<chem>O=C1Cc2cc(Nc3cc(-c4cccs4)ncn3)ccc2N1</chem>	ENAMINE PV-002575796258
	<chem>CC1Cc2cc(CN3C(=O)CN(Cc4ccc5c(c4)CC(=O)N5)C3=O)ccc2O1</chem>	ENAMINE Z3881634056

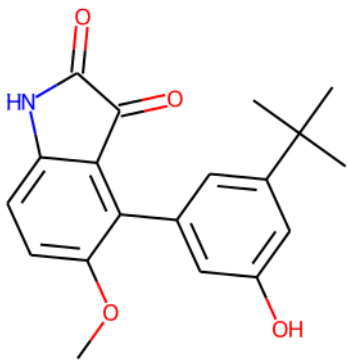
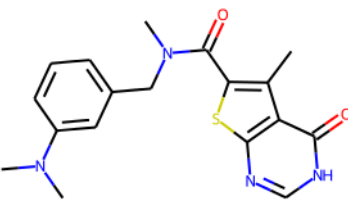
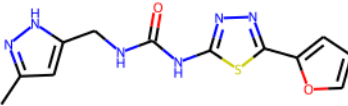
Chemical Structure	SMILES	Vendor
	<chem>CNc1ccc(-c2ccc(S(=O)(=O)NC3CC3)cc2C(=O)O)c1</chem>	ENAMINE PV-003210342906
	<chem>Cc1ccc2c(c1)ncn2CC(=O)OCc1csc(C)c1</chem>	ENAMINE PV-003140900245
	<chem>COc1ccc(C=Cc2ccncc2C2CC2)c1</chem>	ENAMINE PV-003566023845

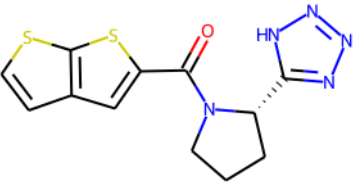
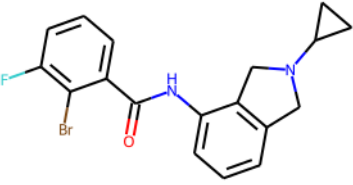
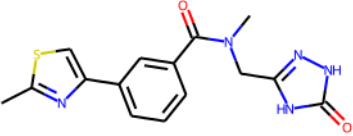
Chemical Structure	SMILES	Vendor
	<chem>CNCc1ccc(OCC(=O)N(C)CC23CC4CC(CC(C4)C2)C3)c1</chem>	ENAMINE PV-003230963807
	<chem>Nc1cc(C(=O)Nc2cccc3c2NC(=O)C3)nn1-c1cc(F)cc1</chem>	ENAMINE PV-003481290237
	<chem>O=C(c1ccccc1-c1ncn[nH]1)N1CCc2c(-c3nn[nH]n3)cccc21</chem>	ENAMINE PV-003200598036


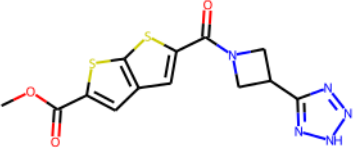
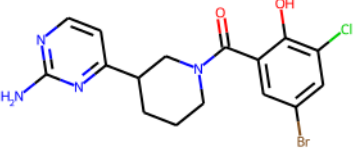
Chemical Structure	SMILES	Vendor
	<chem>CN1CCCC1C(=O)N1CCN(C(=O)c2cc3cc(O)ccc3cc2O)CC1</chem>	ENAMINE Z4310801085
	<chem>COCC(NC(=O)c1cc(=O)n(-c2ccc(Cl)cc2)[nH]1)c1nn[nH]1</chem>	ENAMINE PV-004022354297
	<chem>Cn1c(-c2conc2C2CC2)nc2ccc(F)cc21</chem>	ENAMINE Z3064950344

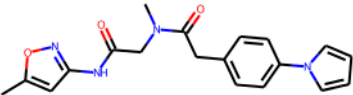
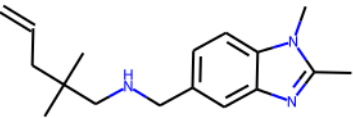
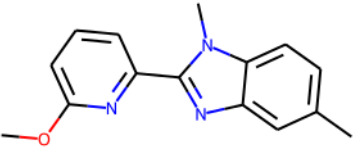
Chemical Structure	SMILES	Vendor
	<chem>CN1CCC1CNC(=O)c1cc(Br)c([N+](=O)[O-])[nH]1</chem>	ENAMINE Z4106716161
	<chem>Cc1ccncc1C(=O)N1CCCC1Cn1c(C)nc2ccccc21</chem>	ENAMINE Z1518010170
	<chem>O=C(c1cncc(-n2cccc2)c1)N1CCc2c(F)cccc21</chem>	ENAMINE PV-002810215700

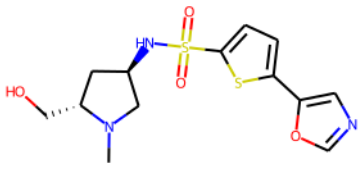
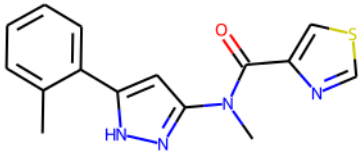
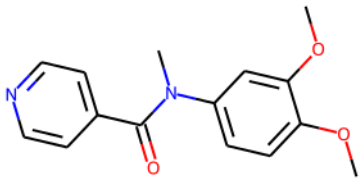
Chemical Structure	SMILES	Vendor
	<chem>Cc1nc2cc(CN[C@H](C)[C@H](C)O)ccc2n1C1CC1</chem>	ENAMINE PV-003266405519
	<chem>CN1C(=O)N(c2ccc3c(c2)NC(=O)C3)C(=O)C12CC2</chem>	ENAMINE Z3349821537
	<chem>CC1CCN(c2ccc(N3C(=O)C(c4ccccc4)N(C)C3=O)cc2)CC1</chem>	ENAMINE Z1891822154

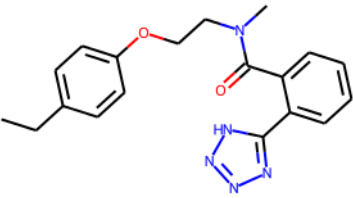
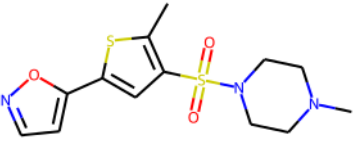
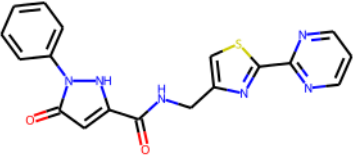
Chemical Structure	SMILES	Vendor
	<chem>COc1ccc2c(c1-c1cc(O)cc(C(C)(C)C)c1)C(=O)C(=O)N2</chem>	ENAMINE Z3548842687
	<chem>Cc1c(C(=O)N(C)Cc2ccc(N(C)C)c2)sc2nc[nH]c(=O)c12</chem>	ENAMINE Z4127267313
	<chem>Cc1cc(CNC(=O)Nc2nnc(-c3ccco3)s2)[nH]n1</chem>	ENAMINE Z1196293325

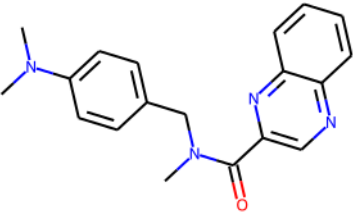
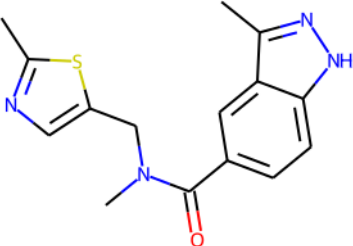
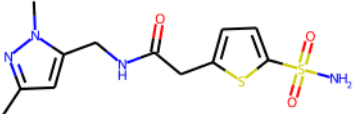
Chemical Structure	SMILES	Vendor
	<chem>O=C(c1cc2ccsc2s1)N1C CC[C@H]1c1nn[nH]1</chem>	ENAMINE Z3205477342
	<chem>O=C(Nc1cccc2c1CN(C1C C1)C2)c1cccc(F)c1Br</chem>	ENAMINE Z2224114638
	<chem>Cc1nc(-c2cccc(C(=O)N (C)Cc3n[nH]c(=O)[nH]3)c2)cs1</chem>	ENAMINE PV-002880489698

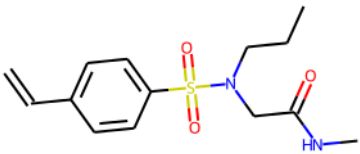
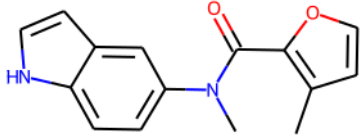
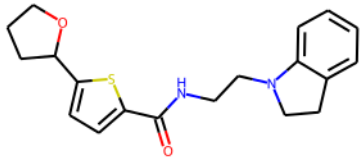
Chemical Structure	SMILES	Vendor
	<chem>CC(=O)c1csc(C(=O)Cn2c(Cl)nc3c2c(=O)n(C)c(=O)n3C)c1</chem>	ENAMINE Z1123846153
	<chem>COC(=O)c1cc2cc(C(=O)N3CC(c4nn[nH]n4)C3)sc2s1</chem>	ENAMINE PV-002951821444
	<chem>Nc1nccc(C2CCCN(C(=O)c3cc(Br)cc(Cl)c3O)C2)n1</chem>	ENAMINE Z2028167249

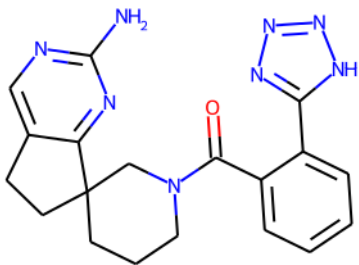
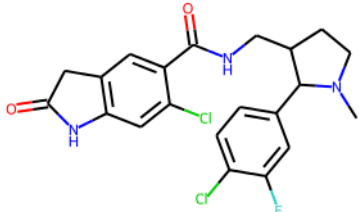
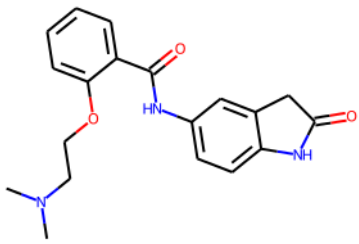
Chemical Structure	SMILES	Vendor
	<chem>Cc1cc(NC(=O)CN(C)C(=O)Cc2ccc(-n3cccc3)cc2)no1</chem>	MCULE MCULE-6150069646
	<chem>C=CCC(C)(C)CNCc1ccc2c(c1)nc(C)n2C</chem>	MCULE MCULE-7115957595
	<chem>COc1cccc(-c2nc3cc(C)ccc3n2C)n1</chem>	MCULE MCULE-8586465316

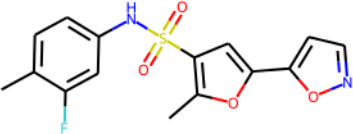
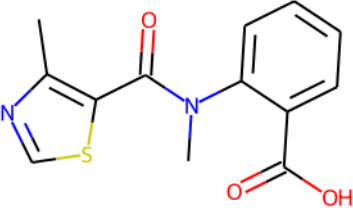
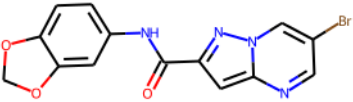
Chemical Structure	SMILES	Vendor
	<chem>CN1C[C@H](NS(=O)(=O)c2ccc(-c3cnco3)s2)C[C@H]1CO</chem>	MCULE MCULE-9325838282
	<chem>Cc1ccccc1-c1cc(N(C)C(=O)c2csn2)n[nH]1</chem>	MCULE MCULE-5814949327
	<chem>COc1ccc(N(C)C(=O)c2ccncc2)cc1OC</chem>	MCULE MCULE-1522978703

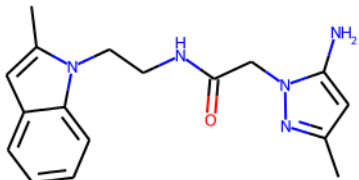
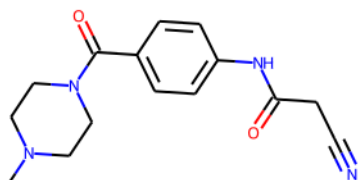
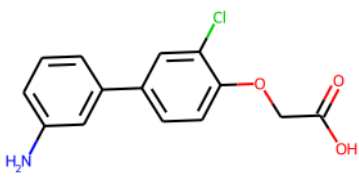
Chemical Structure	SMILES	Vendor
	<chem>CCc1ccc(OCCN(C)C(=O)c2ccccc2-c2nnn[nH]2)cc1</chem>	MCULE MCULE-2743832010
	<chem>Cc1sc(-c2ccno2)cc1S(=O)(=O)N1CCN(C)CC1</chem>	MCULE MCULE-9400880566
	<chem>O=C(NC1csc(-c2ncccn2)n1)c1cc(=O)n(-c2ccccc2)[nH]1</chem>	MCULE MCULE-3296220623

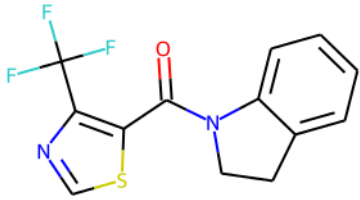
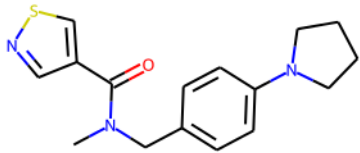
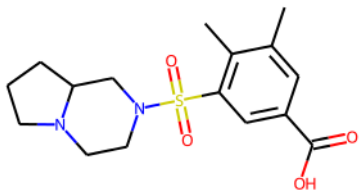
Chemical Structure	SMILES	Vendor
	<chem>CN(Cc1ccc(N(C)C)cc1)C(=O)c1cnc2ccccc2n1</chem>	MCULE MCULE-8689916617
	<chem>Cc1ncc(CN(C)C(=O)c2c3[nH]nc(C)c3c2)s1</chem>	MCULE MCULE-6050272797
	<chem>Cc1cc(CNC(=O)Cc2ccc(S(N)(=O)=O)s2)n(C)n1</chem>	MCULE MCULE-8017248231

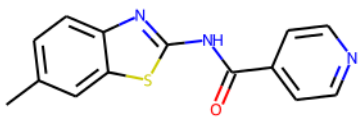
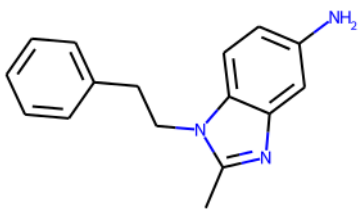
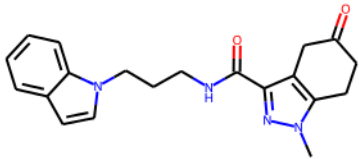
Chemical Structure	SMILES	Vendor
	<chem>C=Cc1ccc(S(=O)(=O)N(CCC)CC(=O)NC)cc1</chem>	MCULE MCULE-6945424310
	<chem>Cc1ccoc1C(=O)N(C)c1ccc2[nH]ccc2c1</chem>	MCULE MCULE-1195499092
	<chem>O=C(NCCN1CCc2ccccc21)c1ccc(C2CCCO2)s1</chem>	MCULE MCULE-4293898923

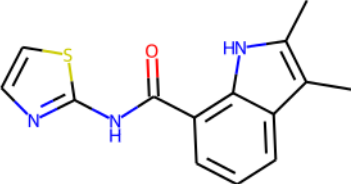
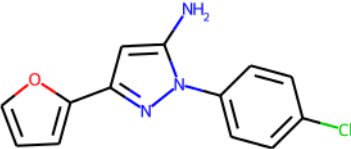
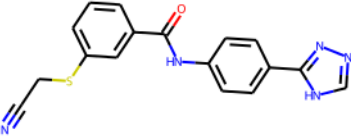
Chemical Structure	SMILES	Vendor
	<chem>Nc1ncc2c(n1)C1(CCCN(C(=O)c3ccccc3-c3nn[nH]3)C1)CC2</chem>	MCULE MCULE-5177075389
	<chem>CN1CCC(CNC(=O)c2cc3c(cc2Cl)NC(=O)C3)C1c1ccc(Cl)c(F)c1</chem>	MCULE MCULE-8184825804
	<chem>CN(C)CCOc1cccc1C(=O)Nc1ccc2c(c1)CC(=O)N2</chem>	MCULE MCULE-1095374120

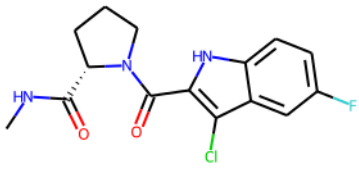
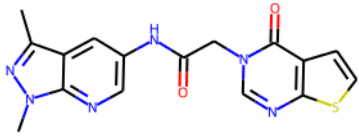
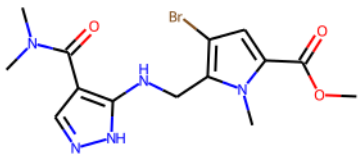
Chemical Structure	SMILES	Vendor
	<chem>Cc1ccc(NS(=O)(=O)c2cc(-c3ccno3)oc2C)cc1F</chem>	MCULE MCULE-3912848812
	<chem>Cc1ncsc1C(=O)N(C)c1ccccc1C(=O)O</chem>	MCULE MCULE-6998860183
	<chem>O=C(Nc1ccc2c(c1)OCO2)c1cc2ncc(Br)cn2n1</chem>	MCULE MCULE-2017133115

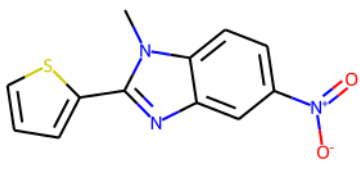
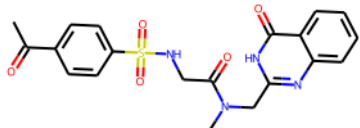
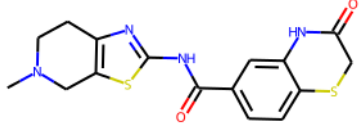
Chemical Structure	SMILES	Vendor
	<chem>Cc1cc(N)n(CC(=O)NCCn2c(C)cc3ccccc32)n1</chem>	MCULE MCULE-6012236602
	<chem>CN1CCN(C(=O)c2ccc(NC(=O)CC#N)cc2)CC1</chem>	MCULE MCULE-4607948790
	<chem>Nc1ccc(-c2ccc(OCC(=O)O)c(Cl)c2)c1</chem>	MCULE MCULE-6250341229

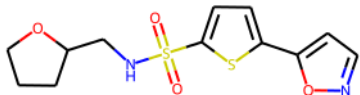
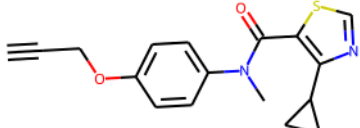
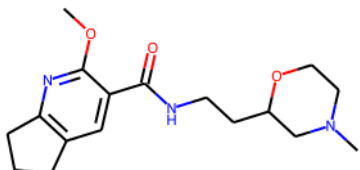
Chemical Structure	SMILES	Vendor
	<chem>O=C(c1scnc1C(F)(F)F)N1CCc2ccccc21</chem>	MCULE MCULE-6555366563
	<chem>CN(Cc1ccc(N2CCCC2)cc1)C(=O)c1cnsc1</chem>	MCULE MCULE-4091995187
	<chem>Cc1cc(C(=O)O)cc(S(=O)(=O)N2CCN3CCCC3C2)c1C</chem>	MCULE MCULE-6843142305

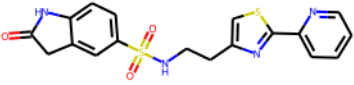
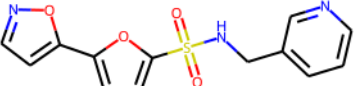
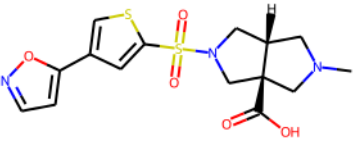
Chemical Structure	SMILES	Vendor
	<chem>Cc1ccc2nc(NC(=O)c3ccncc3)sc2c1</chem>	MCULE MCULE-8297187012
	<chem>Cc1nc2cc(N)ccc2n1CCc1ccccc1</chem>	MCULE MCULE-9679269856
	<chem>Cn1nc(C(=O)NCCCn2ccc3ccccc32)c2c1CCC(=O)C2</chem>	MCULE MCULE-4580753903

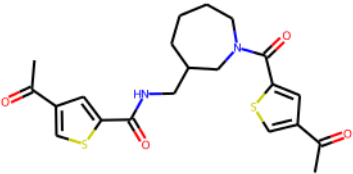
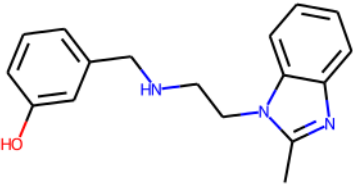
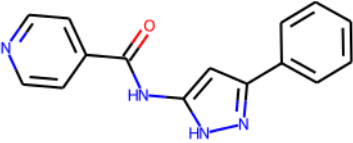
Chemical Structure	SMILES	Vendor
	<chem>Cc1[nH]c2c(C(=O)Nc3nccs3)cccc2c1C</chem>	MCULE MCULE-7167193124
	<chem>Nc1cc(-c2ccco2)nn1-c1ccc(Cl)cc1</chem>	MCULE MCULE-1815956787
	<chem>N#CCSc1cccc(C(=O)Nc2ccc(-c3nnc[nH]3)cc2)c1</chem>	MCULE MCULE-8914597353

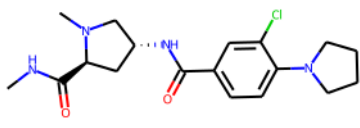
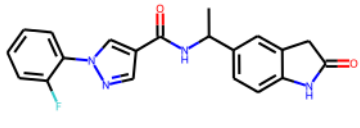
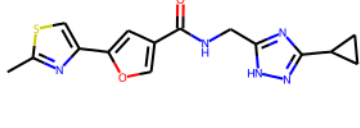
Chemical Structure	SMILES	Vendor
	<chem>CNC(=O)[C@@H]1CCCN1C(=O)c1[nH]c2ccc(F)cc2c1Cl</chem>	MCULE MCULE-2435269564
	<chem>Cc1nn(C)c2ncc(NC(=O)Cn3cnc4sccc4c3=O)cc12</chem>	MCULE MCULE-7777131988
	<chem>COC(=O)c1cc(Br)c(CNc2[nH]ncc2C(=O)N(C)C)n1C</chem>	MCULE MCULE-7413976871

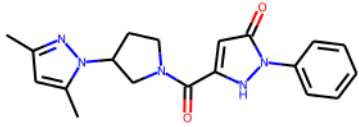
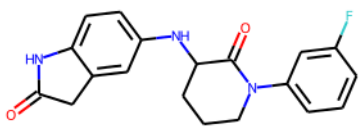
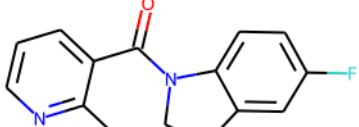
Chemical Structure	SMILES	Vendor
	<chem>Cn1c(-c2cccs2)nc2cc([N+](=O)[O-])ccc21</chem>	MCULE MCULE-3379893590
	<chem>CC(=O)c1ccc(S(=O)(=O)NCC(=O)N(C)Cc2nc3ccc3c(=O)[nH]2)cc1</chem>	MCULE MCULE-4738077028
	<chem>CN1CCc2nc(NC(=O)c3ccc4c(c3)NC(=O)CS4)sc2C1</chem>	MCULE MCULE-5527702335

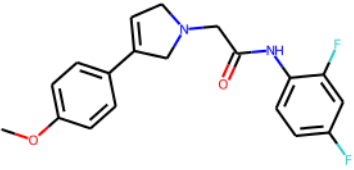
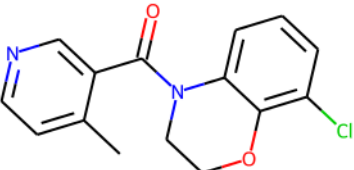
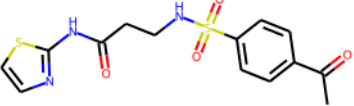
Chemical Structure	SMILES	Vendor
	<chem>O=S(=O)(NCC1CCCO1)c1ccc(-c2ccno2)s1</chem>	MCULE MCULE-5462907469
	<chem>C#CCOc1ccc(N(C)C(=O)c2scnc2C2CC2)cc1</chem>	MCULE MCULE-7053948715
	<chem>COc1nc2c(cc1C(=O)NCCc1ccncc1)ccc2</chem>	MCULE MCULE-5036172124

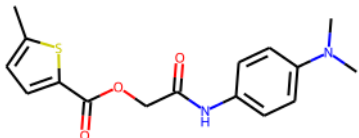
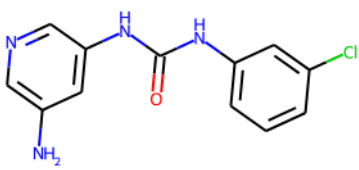
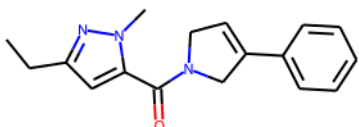
Chemical Structure	SMILES	Vendor
	<chem>O=C1Cc2cc(S(=O)(=O)NCCc3csc(-c4cccn4)n3)ccc2N1</chem>	MCULE MCULE-2380332039
	<chem>O=S(=O)(NCc1cccn1)c1ccc(-c2ccno2)o1</chem>	MCULE MCULE-2786691255
	<chem>CN1C[C@H]2CN(S(=O)(=O)c3cc(-c4ccno4)cs3)C[C@@]2(C(=O)O)C1</chem>	MCULE MCULE-1650012621

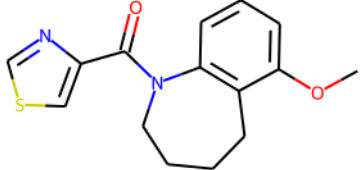
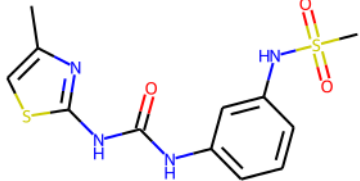
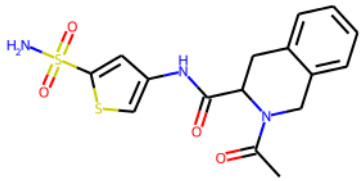
Chemical Structure	SMILES	Vendor
	<chem>CC(=O)c1csc(C(=O)NCC2CCCCN(C(=O)c3cc(C(C)=O)cs3)C2)c1</chem>	MCULE MCULE-3201687388
	<chem>Cc1nc2ccccc2n1CCNCc1ccc(O)c1</chem>	MCULE MCULE-4330145109
	<chem>O=C(Nc1cc(-c2ccccc2)n[nH]1)c1ccncc1</chem>	MCULE MCULE-4093940886

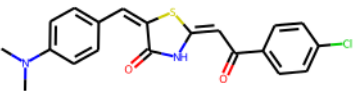
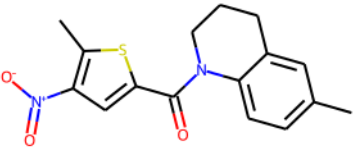
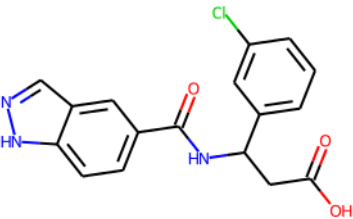
Chemical Structure	SMILES	Vendor
	<chem>CNC(=O)[C@@H]1C[C@@H](NC(=O)c2ccc(N3CCCC3)c(Cl)c2)CN1C</chem>	MCULE MCULE-8707189652
	<chem>CC(NC(=O)c1cnn(-c2ccc(F)c2)c1)c1ccc2c(c1)CC(=O)N2</chem>	MCULE MCULE-1399493626
	<chem>Cc1nc(-c2cc(C(=O)NCc3nc(C4CC4)n[nH]3)co2)cs1</chem>	MCULE MCULE-2720885557

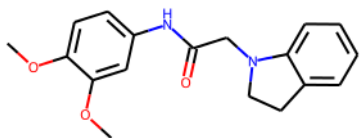
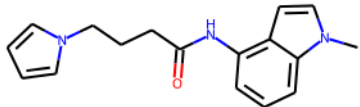
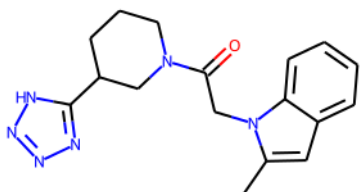
Chemical Structure	SMILES	Vendor
	<chem>Cc1cc(C)n(C2CCN(C(=O)c3cc(=O)n(-c4ccccc4)[nH]3)C2)n1</chem>	MCULE MCULE-9530299198
	<chem>O=C1Cc2cc(NC3CCCN(c4cccc(F)c4)C3=O)ccc2N1</chem>	MCULE MCULE-2995043590
	<chem>Cc1ncccc1C(=O)N1CCc2cc(F)ccc21</chem>	MCULE MCULE-5438026602

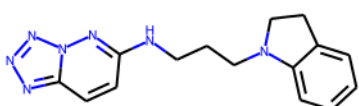
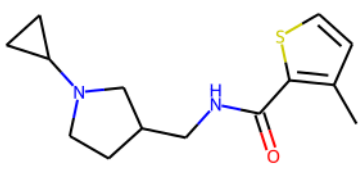
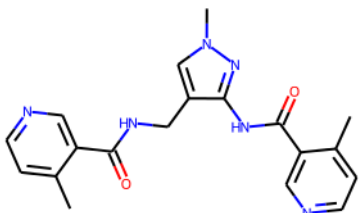
Chemical Structure	SMILES	Vendor
	<chem>COc1ccc(C2=CCN(CC(=O)Nc3ccc(F)cc3F)C2)cc1</chem>	MCULE MCULE-2323044129
	<chem>Cc1ccncc1C(=O)N1CCOc2c(Cl)cccc21</chem>	MCULE MCULE-6176462728
	<chem>CC(=O)c1ccc(S(=O)(=O)NCCC(=O)Nc2nccs2)cc1</chem>	MCULE MCULE-2598280122

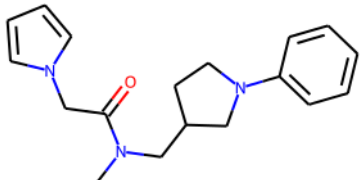
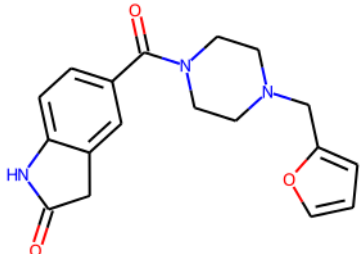
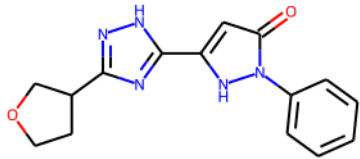
Chemical Structure	SMILES	Vendor
	<chem>Cc1ccc(C(=O)OCC(=O)Nc2ccc(N(C)C)cc2)s1</chem>	MCULE MCULE-7447989007
	<chem>Nc1cncc(NC(=O)Nc2ccc(Cl)cc2)c1</chem>	MCULE MCULE-3786415604
	<chem>CCc1cc(C(=O)N2CC=C(c3ccccc3)C2)n(C)n1</chem>	MCULE MCULE-3724231725

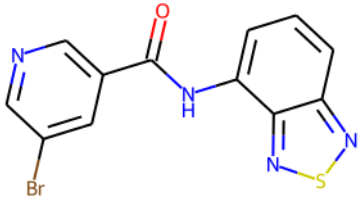
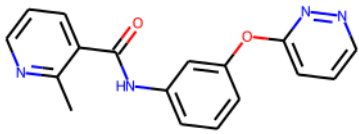
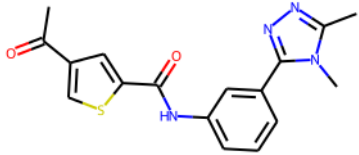
Chemical Structure	SMILES	Vendor
	<chem>COc1cccc2c1CCCCN2C(=O)c1cscn1</chem>	MCULE MCULE-7563140813
	<chem>Cc1csc(NC(=O)Nc2cccc(NS(C)(=O)=O)c2)n1</chem>	MCULE MCULE-7124223667
	<chem>CC(=O)N1Cc2ccccc2CC1C(=O)Nc1csc(S(N)(=O)=O)c1</chem>	MCULE MCULE-6888752150

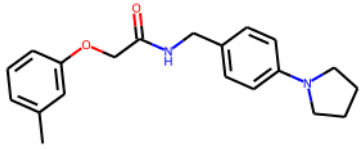
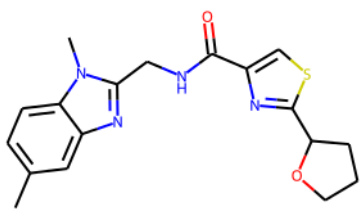
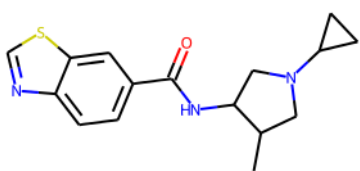
Chemical Structure	SMILES	Vendor
	<chem>CN(C)c1ccc(C=C2SC(=O)NC2=CC(=O)Oc3ccc(Cl)cc3)[nH]c2=O)cc1</chem>	MCULE MCULE-6863881478
	<chem>Cc1ccc2c(c1)CCCN2C(=O)c1cc([N+](=O)[O-])c(C)s1</chem>	MCULE MCULE-4757888907
	<chem>O=C(O)CC(NC(=O)c1ccc2[nH]ncc2c1)c1ccc(Cl)c1</chem>	MCULE MCULE-5363498162

Chemical Structure	SMILES	Vendor
	<chem>COc1ccc(NC(=O)CN2CCc3ccccc32)cc1OC</chem>	MCULE MCULE-2343108955
	<chem>Cn1ccc2c(NC(=O)CCCn3ccccc3)cccc21</chem>	MCULE MCULE-1454664997
	<chem>Cc1cc2ccccc2n1CC(=O)N1CCCC(c2nnn[nH]2)C1</chem>	MCULE MCULE-7049999346

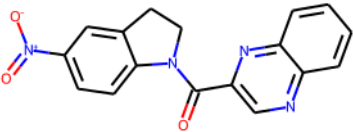
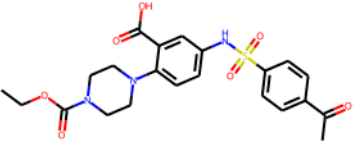
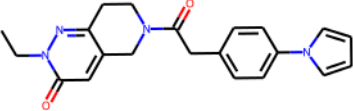
Chemical Structure	SMILES	Vendor
	<chem>c1ccc2c(c1)CCN2CCCNc1ccc2nnnn2n1</chem>	MCULE MCULE-8168758896
	<chem>Cc1ccsc1C(=O)NCC1CCN(C2CC2)C1</chem>	MCULE MCULE-6236935609
	<chem>Cc1ccncc1C(=O)NCc1cn(C)c1NC(=O)c1cnccc1C</chem>	MCULE MCULE-5616699943

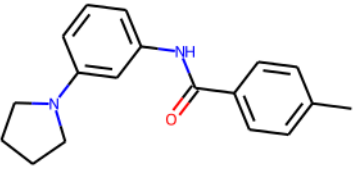
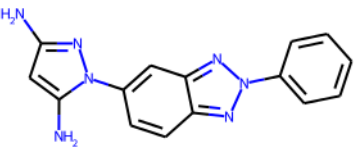
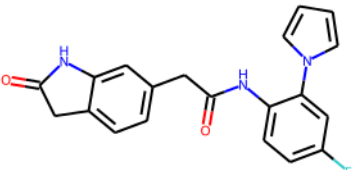
Chemical Structure	SMILES	Vendor
	<chem>CN(CC1CCN(c2ccccc2)C1)C(=O)Cn1cccc1</chem>	MCULE MCULE-3674609563
	<chem>O=C1Cc2cc(C(=O)N3CCN(Cc4ccco4)CC3)ccc2N1</chem>	MCULE MCULE-3121232336
	<chem>O=c1cc(-c2nc(C3CCOC3)n[nH]2)[nH]n1-c1ccccc1</chem>	MCULE MCULE-9181613779

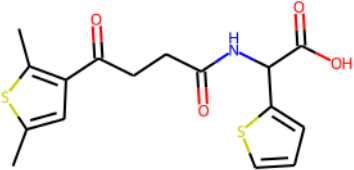
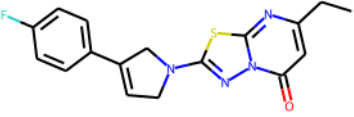
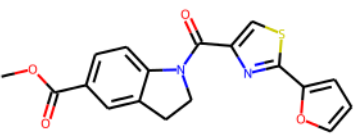
Chemical Structure	SMILES	Vendor
	<chem>O=C(Nc1cccc2nsnc12)c1cncc(Br)c1</chem>	MCULE MCULE-2007654396
	<chem>Cc1ncccc1C(=O)Nc1ccc(Oc2cccn2)c1</chem>	MCULE MCULE-8962491230
	<chem>CC(=O)c1csc(C(=O)Nc2ccc(-c3nnc(C)n3C)c2)c1</chem>	MCULE MCULE-9895096722

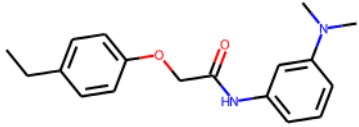
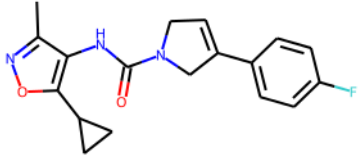
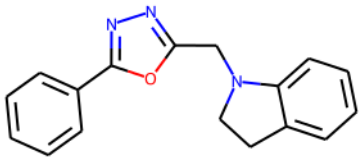
Chemical Structure	SMILES	Vendor
	<chem>Cc1ccc(OCC(=O)NCc2ccc(N3CCCC3)cc2)c1</chem>	MCULE MCULE-3236808541
	<chem>Cc1ccc2c(c1)nc(CNC(=O)c3csc(C4CCCCO4)n3)n2C</chem>	MCULE MCULE-8235111625
	<chem>CC1CN(C2CC2)CC1NC(=O)c3ccc4ncsc4c3</chem>	MCULE MCULE-5289471275

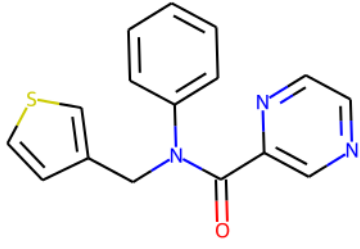
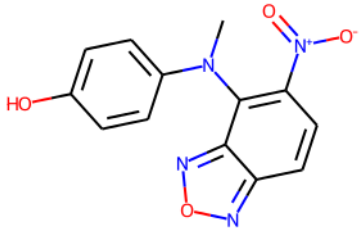
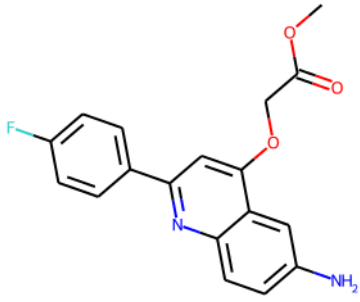
Chemical Structure	SMILES	Vendor
	<chem>O=C1Cc2cc(CNc3ccnc(-c4ccc(O)c4)n3)ccc2N1</chem>	MCULE MCULE-9886412635
	<chem>COc1ccc(-c2cc(=O)n(-c3ccc(C)c3)[nH]2)cc1OC</chem>	MCULE MCULE-5332250826
	<chem>COc1cccc(C2=CCN(C(=O)NCC(F)(F)F)C2)c1</chem>	MCULE MCULE-9732566775

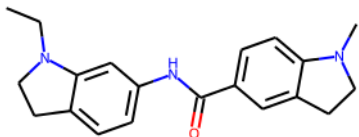
Chemical Structure	SMILES	Vendor
	<chem>O=C(c1cnc2ccccc2n1)N1CCc2cc([N+](=O)[O-])ccc21</chem>	MCULE MCULE-5867929098
	<chem>CCOC(=O)N1CCN(c2ccc(NS(=O)(=O)c3ccc(C(C)=O)cc3)cc2C(=O)O)CC1</chem>	MCULE MCULE-2525248838
	<chem>CCn1nc2c(cc1=O)CN(C(=O)Cc1ccc(-n3cccc3)cc1)CC2</chem>	MCULE MCULE-5615564347

Chemical Structure	SMILES	Vendor
	<chem>Cc1ccc(C(=O)Nc2ccc(N3CCCC3)cc2)cc1</chem>	MCULE MCULE-9937637288
	<chem>Nc1cc(N)n(-c2ccc3nn(-c4cccc4)nc3c2)n1</chem>	MCULE MCULE-5527970470
	<chem>O=C1Cc2ccc(CC(=O)Nc3ccc(F)cc3-n3cccc3)cc2N1</chem>	MCULE MCULE-3165530075

Chemical Structure	SMILES	Vendor
	<chem>Cc1cc(C(=O)CCC(=O)NC(=O)O)c2cccs2)c(C)s1</chem>	MCULE MCULE-1446861798
	<chem>CCc1cc(=O)n2nc(N3CC=C(c4ccc(F)cc4)C3)sc2n1</chem>	MCULE MCULE-4970180752
	<chem>COC(=O)c1ccc2c(c1)CCN2C(=O)c1csc(-c2ccco2)n1</chem>	MCULE MCULE-6045346838

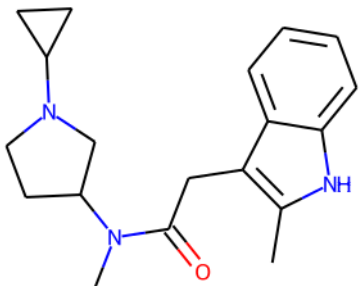
Chemical Structure	SMILES	Vendor
	<chem>CCc1ccc(OCC(=O)Nc2ccc(N(C)C)cc2)cc1</chem>	MCULE MCULE-4141511012
	<chem>Cc1noc(C2CC2)c1NC(=O)N1CC=C(c2ccc(F)cc2)C1</chem>	MCULE MCULE-4829702189
	<chem>c1ccc(-c2nnc(CN3CCc4ccccc43)o2)cc1</chem>	MCULE MCULE-6487584352

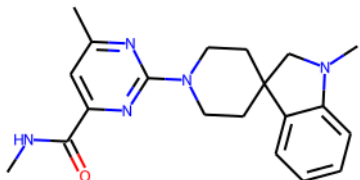
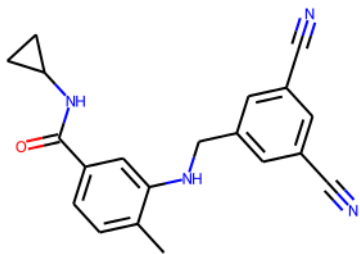
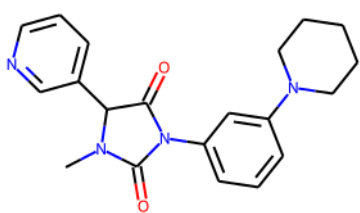
Chemical Structure	SMILES	Vendor
	<chem>O=C(c1cnccn1)N(Cc1ccsc1)c1ccccc1</chem>	MCULE MCULE-3841490358
	<chem>CN(c1ccc(O)cc1)c1c([N+](=O)[O-])ccc2nnc12</chem>	MCULE MCULE-3716980606
	<chem>COC(=O)COc1cc(-c2ccc(F)cc2)nc2ccc(N)cc12</chem>	MCULE MCULE-1786282016

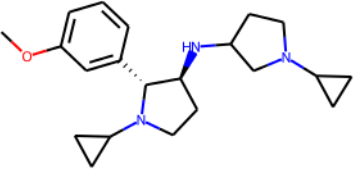
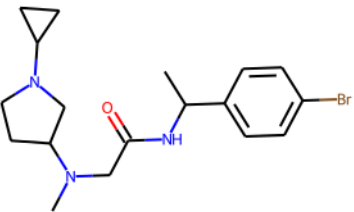
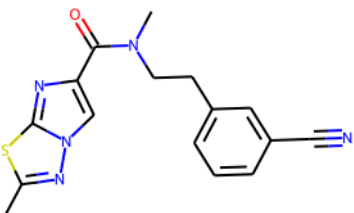
Chemical Structure	SMILES	Vendor
	<chem>CCN1CCc2ccc(NC(=O)c3ccc4c(c3)CCN4C)cc21</chem>	MCULE MCULE-7770518221

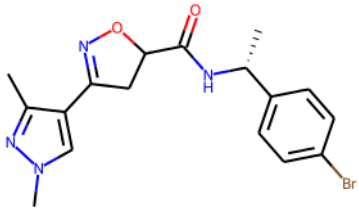
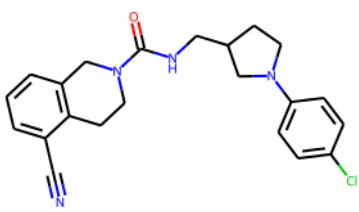
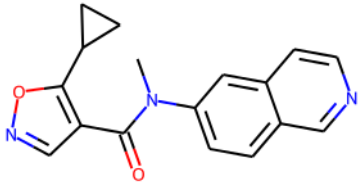
3 WDR91

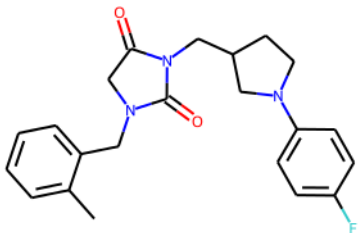
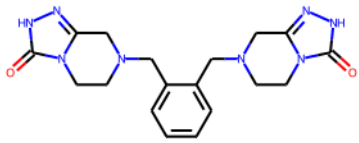
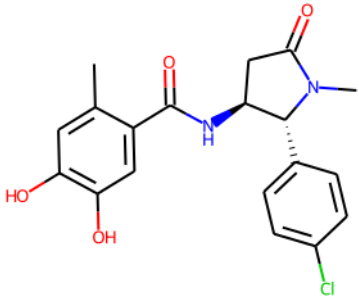
UniProtKB entry A4D1P6

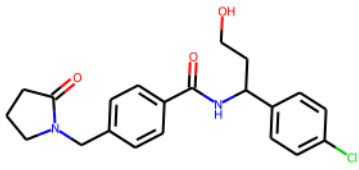
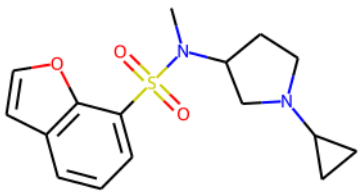
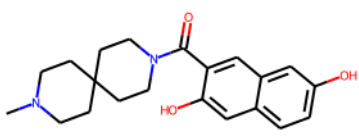
Chemical Structure	SMILES	Vendor
	<chem>Cc1[nH]c2ccccc2c1CC(=O)N(C)C1CCN(C2CC2)C1</chem>	ENAMINE Z1173513225

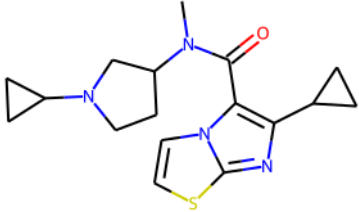
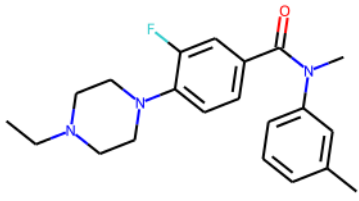
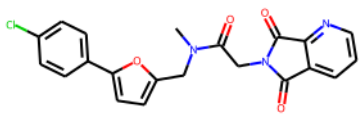
Chemical Structure	SMILES	Vendor
	<chem>CNC(=O)c1cc(C)nc(N2C CC3(CC2)CN(C)c2cccc23)n1</chem>	ENAMINE Z3833649758
	<chem>Cc1ccc(C(=O)NC2CC2)c c1NCc1cc(C#N)cc(C#N)c1</chem>	ENAMINE Z3860190201
	<chem>CN1C(=O)N(c2cccc(N3C CCCC3)c2)C(=O)C1c1ccnc1</chem>	ENAMINE Z2928943147

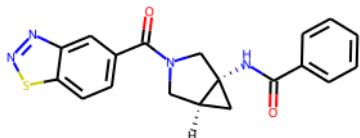
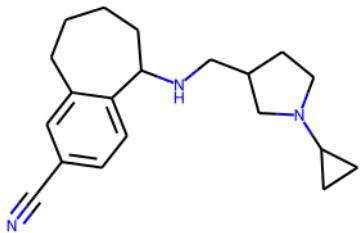
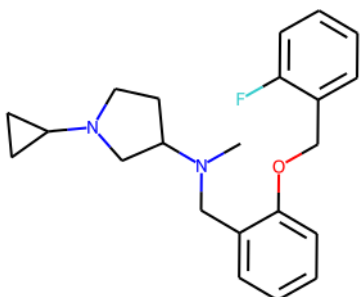
Chemical Structure	SMILES	Vendor
	<chem>COc1cccc([C@@H]2[C@@H](NC3CCN(C4CC4)C3)C(CN2C2CC2)c1</chem>	ENAMINE Z3362613086
	<chem>CC(NC(=O)CN(C)C1CCN(C2CC2)C1)c1ccc(Br)cc1</chem>	ENAMINE Z1176729393
	<chem>Cc1nn2cc(C(=O)N(C)CCc3ccc(C#N)cc3)nc2s1</chem>	ENAMINE Z3360825320

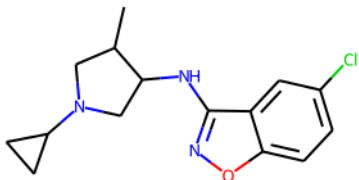
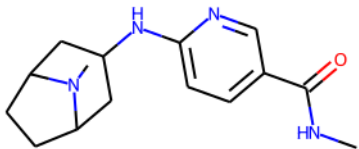
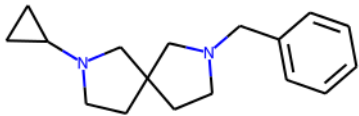
Chemical Structure	SMILES	Vendor
	<chem>Cc1nn(C)cc1C1=NOC(C(=O)N[C@H](C)c2ccc(Br)cc2)C1</chem>	ENAMINE Z2959083512
	<chem>N#Cc1cccc2c1CCN(C(=O)NCC1CCN(c3ccc(Cl)cc3)C1)C2</chem>	ENAMINE Z2199609349
	<chem>CN(C(=O)c1cnoc1C1CC1)c1ccc2cnccc2c1</chem>	ENAMINE PV-003539871062

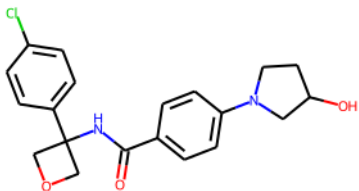
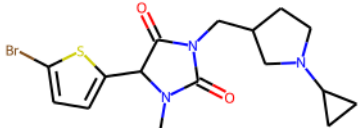
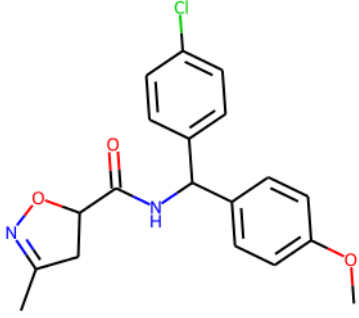
Chemical Structure	SMILES	Vendor
	<chem>Cc1ccccc1CN1CC(=O)N(CC2CCN(c3ccc(F)cc3)C2)C1=O</chem>	ENAMINE Z1868937816
	<chem>O=c1[nH]nc2n1CCN(Cc1ccccc1CN1CCn3c(n[nH]c3=O)C1)C2</chem>	ENAMINE Z1723157813
	<chem>Cc1cc(O)c(O)cc1C(=O)N[C@H]1CC(=O)N(C)[C@@H]1c1ccc(Cl)cc1</chem>	ENAMINE Z4294387454

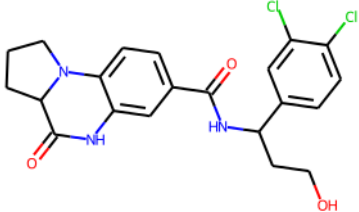
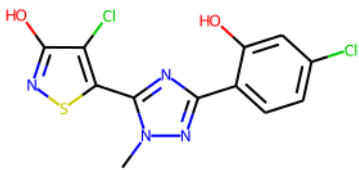
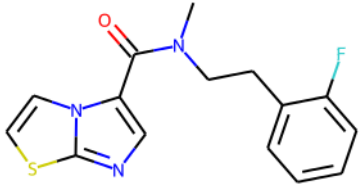
Chemical Structure	SMILES	Vendor
	<chem>O=C(NC(CCO)c1ccc(Cl)cc1)c1ccc(CN2CCCC2=O)cc1</chem>	ENAMINE Z2200611484
	<chem>CN(C1CCN(C2CC2)C1)S(=O)(=O)c1cccc2ccoc12</chem>	ENAMINE Z2276312774
	<chem>CN1CCC2(CC1)CCN(C(=O)c1cc3cc(O)ccc3cc1O)CC2</chem>	ENAMINE Z4311823359

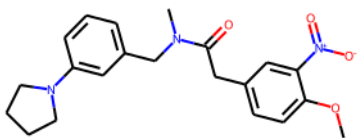
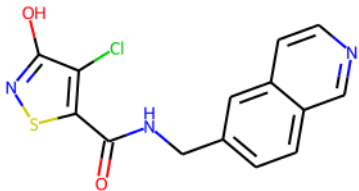
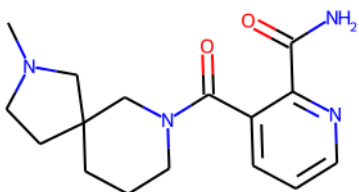
Chemical Structure	SMILES	Vendor
	<chem>CN(C(=O)c1c(C2CC2)nc2scn12)C1CCN(C2CC2)C1</chem>	ENAMINE Z1481478680
	<chem>CCN1CCN(c2ccc(C(=O)N(C)c3ccc(C)cc3)cc2F)CC1</chem>	ENAMINE Z1048477424
	<chem>CN(Cc1ccc(-c2ccc(Cl)cc2)o1)C(=O)CN1C(=O)c2cccnc2C1=O</chem>	ENAMINE Z1167420839

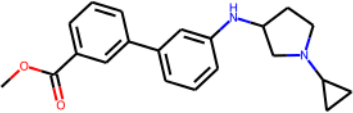
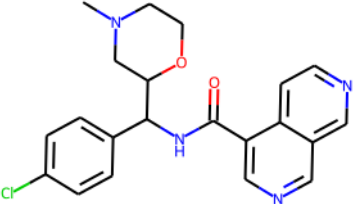
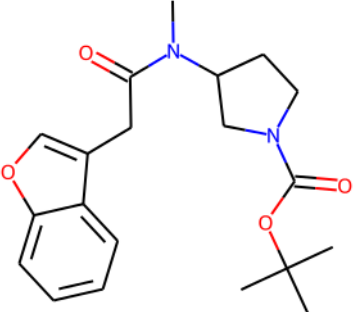
Chemical Structure	SMILES	Vendor
	<chem>O=C(N[C@]12C[C@H]1CN(C(=O)c1ccc3snnc3c1)C2)c1ccccc1</chem>	ENAMINE PV-004035314428
	<chem>N#Cc1ccc2c(c1)CCCCC2NCC1CCN(C2CC2)C1</chem>	ENAMINE Z1959918356
	<chem>CN(Cc1ccccc1OCc1ccccc1F)C1CCN(C2CC2)C1</chem>	ENAMINE PV-003389480707

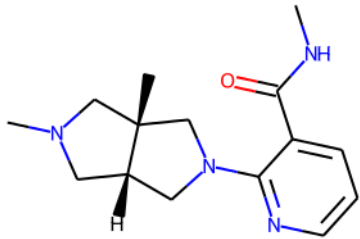
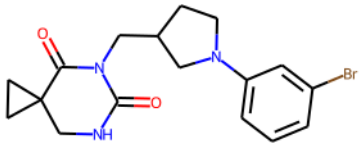
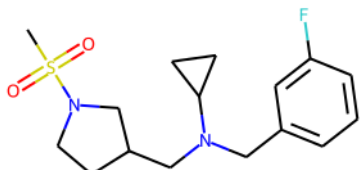
Chemical Structure	SMILES	Vendor
	<chem>CC1CN(C2CC2)CC1Nc1no</chem> <chem>c2ccc(Cl)cc12</chem>	ENAMINE PV-003400327129
	<chem>CNC(=O)c1ccc(NC2CC3C</chem> <chem>CC(C2)N3C)nc1</chem>	ENAMINE Z2274141778
	<chem>c1ccc(CN2CCC3(CC(C4</chem> <chem>CC4)C3)C2)cc1</chem>	ENAMINE Z4265950420

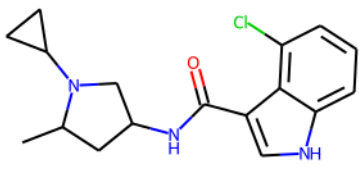
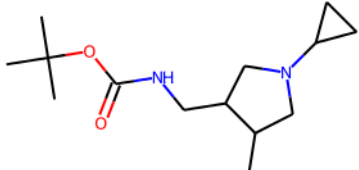
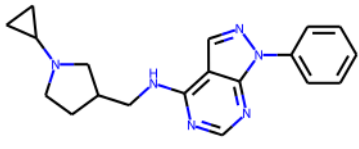
Chemical Structure	SMILES	Vendor
	<chem>O=C(NC1(c2ccc(Cl)cc2)COC1)c1ccc(N2CCC(O)C2)cc1</chem>	ENAMINE Z4305885019
	<chem>CN1C(=O)N(CC2CCN(C3CC3)C2)C(=O)C1c1ccc(Br)s1</chem>	ENAMINE Z2768995516
	<chem>COc1ccc(C(NC(=O)C2CC(C)=NO2)c2ccc(Cl)cc2)cc1</chem>	ENAMINE PV-002312771828

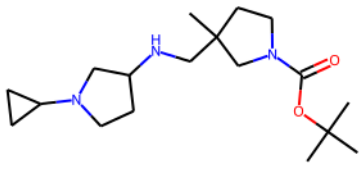
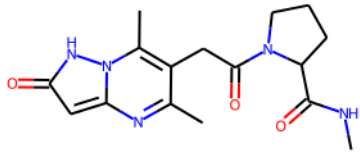
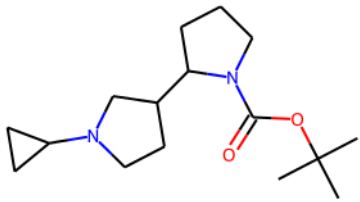
Chemical Structure	SMILES	Vendor
	<chem>O=C(NC(CCO)c1ccc(Cl)c(Cl)c1)C1CCCN21</chem>	ENAMINE Z2091422650
	<chem>Cn1nc(-c2ccc(Cl)cc2O)nc1-c1snc(O)c1Cl</chem>	ENAMINE PV-003186771519
	<chem>CN(CCc1ccccc1F)C(=O)c1cnc2sccn12</chem>	ENAMINE PV-002486366618

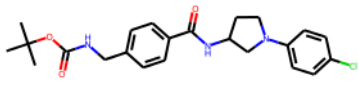
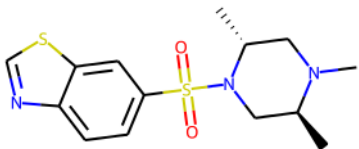
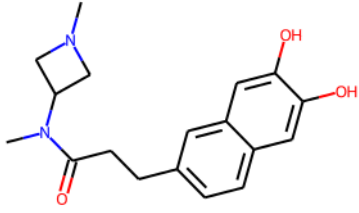
Chemical Structure	SMILES	Vendor
	<chem>COc1ccc(CC(=O)N(C)Cc2ccc([N+](=O)[O-])cc2)cc1</chem>	ENAMINE Z2966813285
	<chem>O=C(NCc1ccc2cnccc2c1)c1snc(O)c1Cl</chem>	ENAMINE PV-003527638947
	<chem>CN1CCC2(CCCN(C(=O)c3ccnc3C(N)=O)C2)C1</chem>	ENAMINE Z2640810955

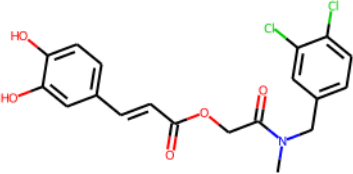
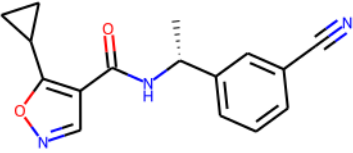
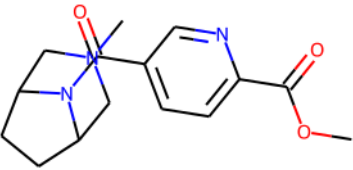
Chemical Structure	SMILES	Vendor
	<chem>COC(=O)c1cccc(-c2ccc(NC3CCN(C4CC4)C3)c2)c1</chem>	ENAMINE PV-003001562235
	<chem>CN1CCOC(C(NC(=O)c2cnc3cnc23)c2ccc(Cl)cc2)C1</chem>	ENAMINE Z4382778396
	<chem>CN(C(=O)Cc1coc2ccccc12)C1CCN(C(=O)OC(C)(C)C)C1</chem>	ENAMINE Z2072050704

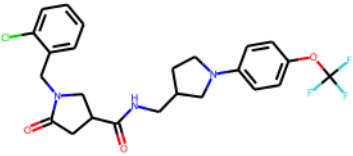
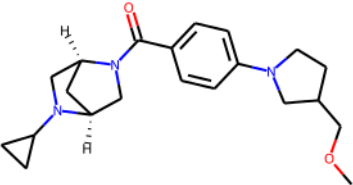
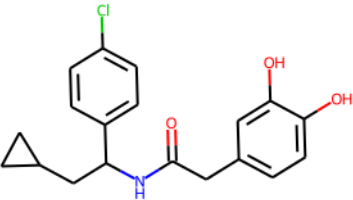
Chemical Structure	SMILES	Vendor
	<chem>CNC(=O)c1ccnc1N1C[C@@H]2CN(C)C[C@]2(C)C1</chem>	ENAMINE Z2976563848
	<chem>O=C1NCC2(CC2)C(=O)N1CC1CCN(c2cccc(Br)c2)C1</chem>	ENAMINE Z3210929701
	<chem>CS(=O)(=O)N1CCC(CN(Cc2cccc(F)c2)C2CC2)C1</chem>	ENAMINE Z2015132115

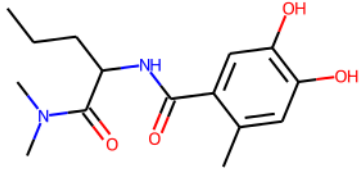
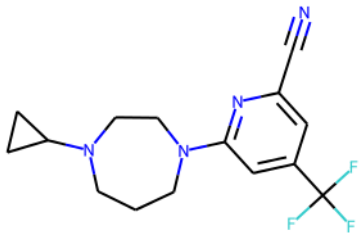
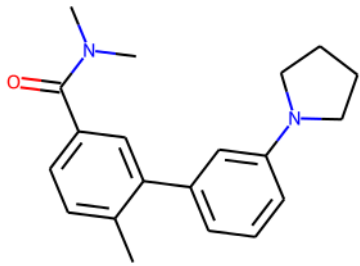
Chemical Structure	SMILES	Vendor
	<chem>CC1CC(NC(=O)c2c[nH]c3ccccc3c2)CN1C1CC1</chem>	ENAMINE Z4123016998
	<chem>CC1CN(C2CC2)CC1CNC(=O)OC(C)(C)C</chem>	ENAMINE Z4267892959
	<chem>c1ccc(-n2ncc3c(NCC4C5CN(C5CC5)C4)ncc32)cc1</chem>	ENAMINE Z397791294

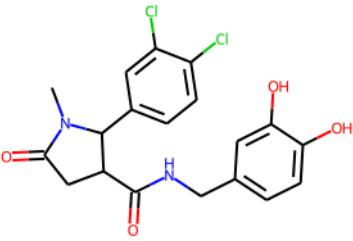
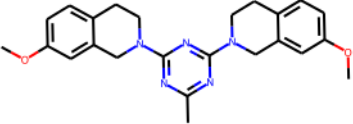
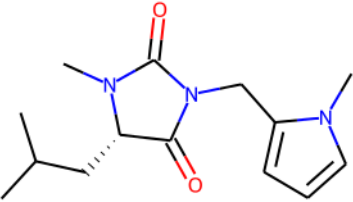
Chemical Structure	SMILES	Vendor
	<chem>CC1(CNC2CCN(C3CC3)C2)CCN(C(=O)OC(C)(C)C)C1</chem>	ENAMINE Z1986719890
	<chem>CNC(=O)C1CCCN1C(=O)Cc1c(C)nc2cc(=O)[nH]n2c1C</chem>	ENAMINE Z1162660401
	<chem>CC(C)(C)OC(=O)N1CCCC1C1CCN(C2CC2)C1</chem>	ENAMINE Z4268743041

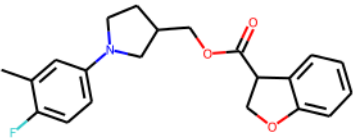
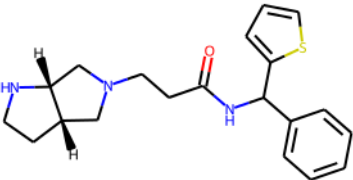
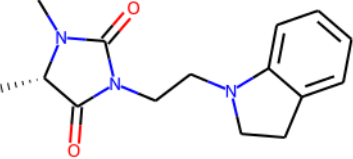
Chemical Structure	SMILES	Vendor
	<chem>CC(C)(C)OC(=O)NCc1ccc(C(=O)NC2CCN(c3ccc(Cl)cc3)C2)cc1</chem>	ENAMINE Z1602038317
	<chem>C[C@H]1CN(S(=O)(=O)c2ccc3ncsc3c2)[C@H](C)CN1C</chem>	ENAMINE PV-003671064753
	<chem>CN1CC(N(C)C(=O)CCc2c3cc(O)c(O)cc3c2)C1</chem>	ENAMINE Z4325243054

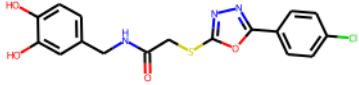
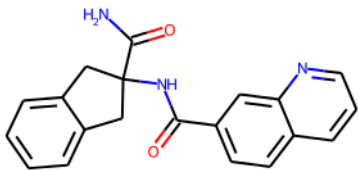
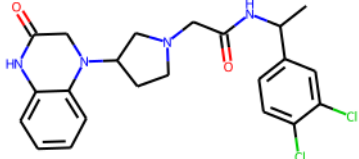
Chemical Structure	SMILES	Vendor
	<chem>CN(Cc1ccc(Cl)c(Cl)c1)C(=O)COC(=O)C=Cc1ccc(O)c(O)c1</chem>	ENAMINE Z1476738797
	<chem>C[C@@H](NC(=O)c1cnoc1C1CC1)c1cccc(C#N)c1</chem>	ENAMINE Z3918821762
	<chem>COC(=O)c1ccc(C(=O)N2C3CCC2CN(C)C3)cn1</chem>	ENAMINE Z2916159340

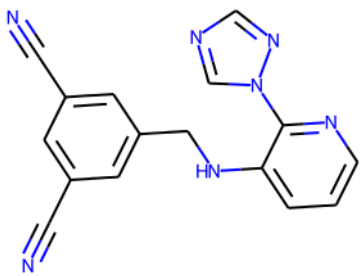
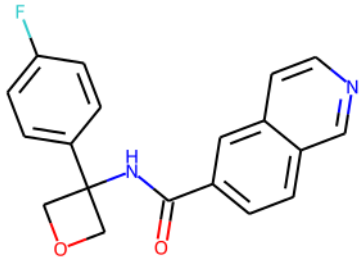
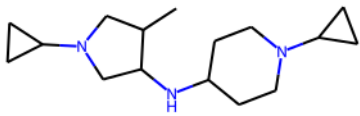
Chemical Structure	SMILES	Vendor
	<chem>O=C(NCC1CCN(c2ccc(OC(F)(F)F)cc2)C1)CC(=O)N(Cc2ccccc2Cl)C1</chem>	ENAMINE Z872738504
	<chem>COCC1CCN(c2ccc(C(=O)N3C[C@@H]4C[C@H]3CN4C3CC3)cc2)C1</chem>	ENAMINE Z4199892951
	<chem>O=C(Cc1ccc(O)c(O)c1)NC(CC1CC1)c1ccc(Cl)cc1</chem>	ENAMINE Z3630941352

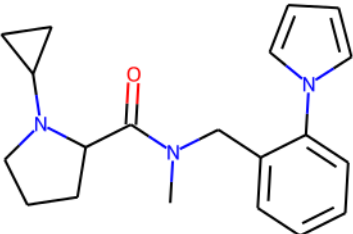
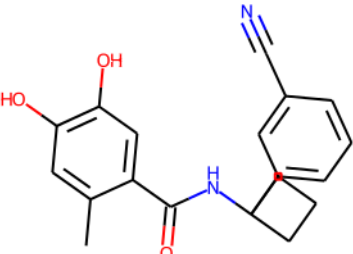

Chemical Structure	SMILES	Vendor
	<chem>CCCC(NC(=O)c1cc(O)c(C)cc1C)C(=O)N(C)C</chem>	ENAMINE Z4295831506
	<chem>N#Cc1cc(C(F)(F)F)cc(N2CCCN(C3CC3)CC2)n1</chem>	ENAMINE Z2769605576
	<chem>Cc1ccc(C(=O)N(C)C)cc1-c1cccc(N2CCCC2)c1</chem>	ENAMINE Z4414837755

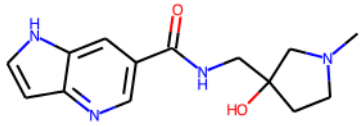
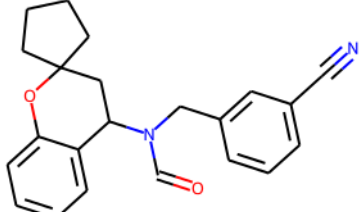
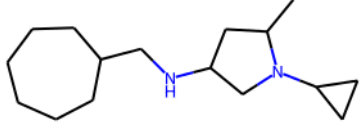
Chemical Structure	SMILES	Vendor
	<chem>CN1C(=O)CC(C(=O)NCc2ccc(O)c(O)c2)C1c1ccc(Cl)c(Cl)c1</chem>	ENAMINE Z1840405448
	<chem>COc1ccc2c(c1)CN(c1nc(C)nc(N3CCc4ccc(OC)cc4C3)n1)CC2</chem>	ENAMINE Z1730755754
	<chem>CC(C)C[C@H]1C(=O)N(Cc2cccn2C)C(=O)N1C</chem>	ENAMINE Z2205790339

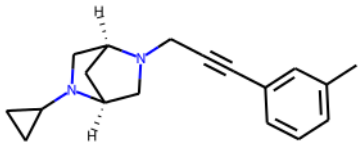
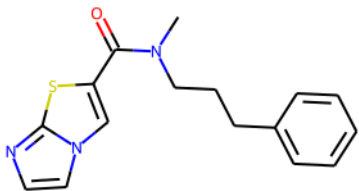
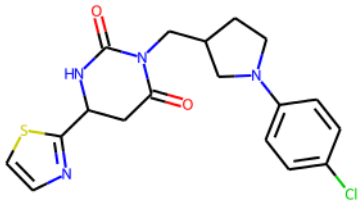
Chemical Structure	SMILES	Vendor
	<chem>Cc1cc(N2CCC(COC(=O)C3COC4ccccc43)C2)ccc1F</chem>	ENAMINE PV-002720143416
	<chem>O=C(CCN1C[C@@H]2CCN[C@@H]2C1)NC(c1ccccc1)c1cccs1</chem>	ENAMINE Z4392244669
	<chem>C[C@H]1C(=O)N(CCN2CCc3ccccc32)C(=O)N1C</chem>	ENAMINE Z2926270736

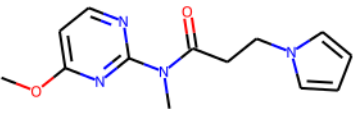
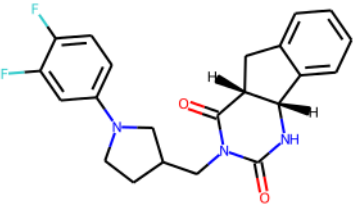
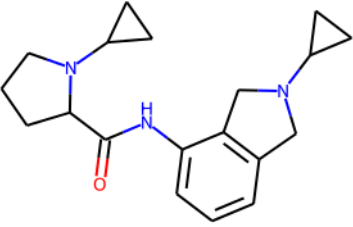
Chemical Structure	SMILES	Vendor
	<chem>O=C(CSc1nnc(-c2ccc(Cl)cc2)o1)NCc1ccc(O)c(O)c1</chem>	ENAMINE Z1451207994
	<chem>NC(=O)C1(NC(=O)c2ccc3ccncc3c2)Cc2ccccc2C1</chem>	ENAMINE PV-002316846068
	<chem>CC(NC(=O)CN1CCC(N2CC(=O)Nc3ccccc32)C1)c1ccc(Cl)c(Cl)c1</chem>	ENAMINE Z1677476919

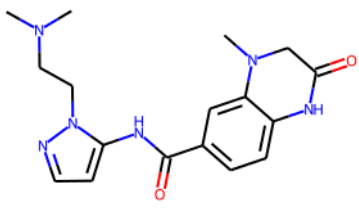
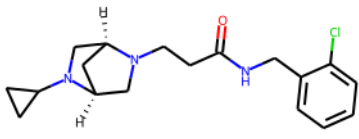
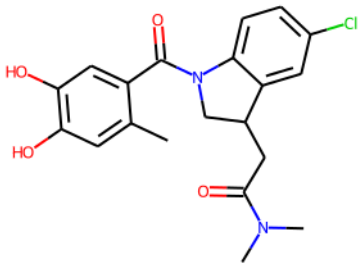
Chemical Structure	SMILES	Vendor
	<chem>N#Cc1cc(C#N)cc(CNc2ccncc2)c1</chem>	ENAMINE PV-002910860062
	<chem>O=C(NC1(c2ccc(F)cc2)COC1)c1ccc2cnc2c1</chem>	ENAMINE PV-002309973688
	<chem>CC1CN(C2CC2)CC1NC1CCN(C2CC2)CC1</chem>	ENAMINE Z1620502552

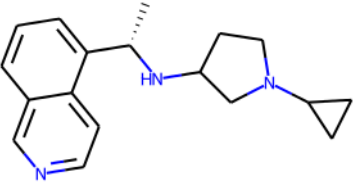
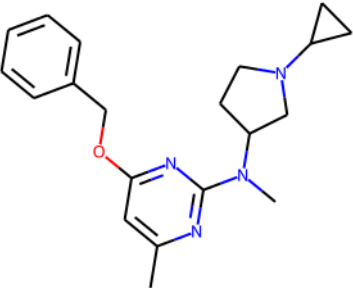
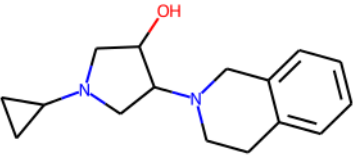
Chemical Structure	SMILES	Vendor
	<chem>CN(Cc1ccccc1-n1cccc1)C(=O)C1CCCN1C1CC1</chem>	ENAMINE PV-002199163365
	<chem>Cc1cc(O)c(O)cc1C(=O)NC1(c2cccc(C#N)c2)CCC1</chem>	ENAMINE Z4292556414
	<chem>O=C(NC(CO)C(O)c1ccc(Cl)cc1)c1ccc2ccncc2c1</chem>	ENAMINE PV-002946257533

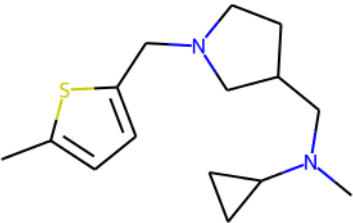
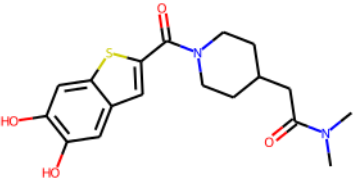
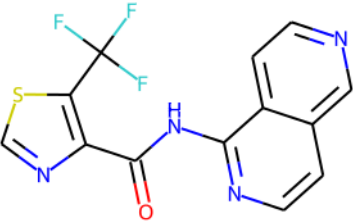
Chemical Structure	SMILES	Vendor
	<chem>CN1CCC(O)(CNC(=O)c2cnc3cc[nH]c3c2)C1</chem>	ENAMINE Z2839747305
	<chem>N#Cc1cccc(CN(C=O)C2C3(CCCC3)Oc3ccccc32)c1</chem>	ENAMINE Z4355077279
	<chem>CC1CC(NCC2CCCCC2)CN1C1CC1</chem>	ENAMINE Z1381788194

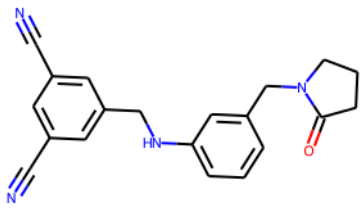
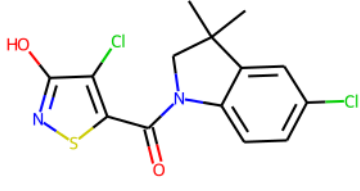
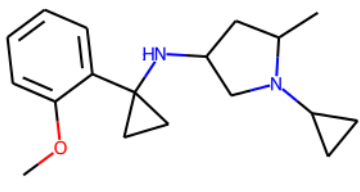
Chemical Structure	SMILES	Vendor
	<chem>Cc1ccc(C#CCN2C[C@@H]3C[C@H]2CN3C2CC2)c1</chem>	ENAMINE Z4314882867
	<chem>CN(CCCC1=CC=CC=C1)C(=O)c1cn2ccnc2s1</chem>	ENAMINE Z1796089026
	<chem>O=C1CC(c2nccs2)NC(=O)N1CC1CCN(c2ccc(Cl)cc2)C1</chem>	ENAMINE Z3426114111

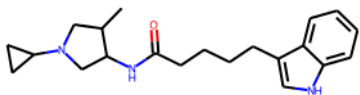
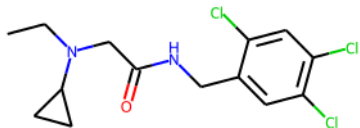
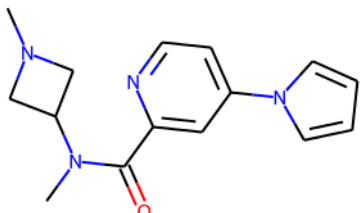
Chemical Structure	SMILES	Vendor
	<chem>COc1ccnc(N(C)C(=O)CCn2ccccc2)n1</chem>	ENAMINE Z2493735547
	<chem>O=C1N[C@H]2c3ccccc3C[C@H]2C(=O)N1CC1CCN(c2ccc(F)c(F)c2)C1</chem>	ENAMINE Z3463128149
	<chem>O=C(Nc1cccc2c1CN(C1CC1)C2)C1CCCN1C1CC1</chem>	ENAMINE Z1906852141

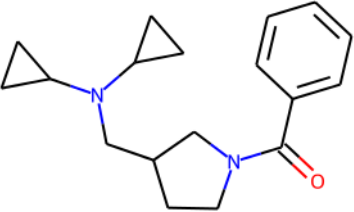
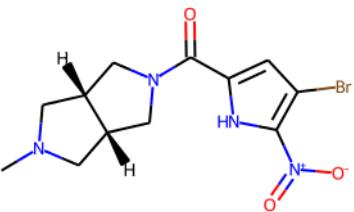
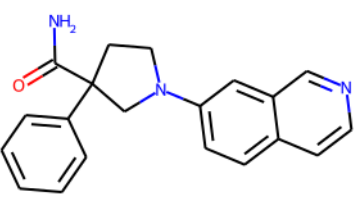
Chemical Structure	SMILES	Vendor
	<chem>CN(C)CCn1nccc1NC(=O)c1ccc2c(c1)N(C)CC(=O)N2</chem>	ENAMINE Z4642093215
	<chem>O=C(CCN1C[C@@H]2C[C@H]1CN2C1CC1)NCc1ccccc1Cl</chem>	ENAMINE Z4194213283
	<chem>Cc1cc(O)c(O)cc1C(=O)N1CC(CC(=O)N(C)C)c2cc(Cl)ccc21</chem>	ENAMINE Z4288918954

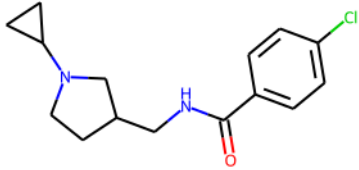
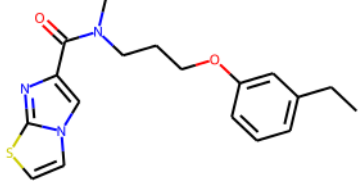
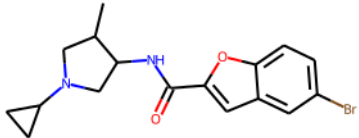
Chemical Structure	SMILES	Vendor
	<chem>C[C@H](NC1CCN(C2CC2)C1)c1cccc2cnccc12</chem>	ENAMINE Z3363535488
	<chem>Cc1cc(OCc2ccccc2)nc(N(C)C2CCN(C3CC3)C2)n1</chem>	ENAMINE PV-002577828875
	<chem>OC1CN(C2CC2)CC1N1CCc2ccccc2C1</chem>	ENAMINE Z3410220640

Chemical Structure	SMILES	Vendor
	<chem>Cc1ccc(CN2CCCC(CN(C)C3CC3)C2)s1</chem>	ENAMINE Z4265702894
	<chem>CN(C)C(=O)CC1CCN(C(=O)c2cc3cc(O)c(O)cc3s2)CC1</chem>	ENAMINE Z2879827538
	<chem>O=C(Nc1nccc2cnccc12)c1ncsc1C(F)(F)F</chem>	ENAMINE PV-002963310838

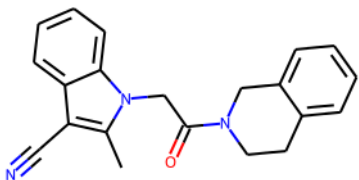
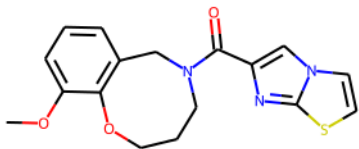
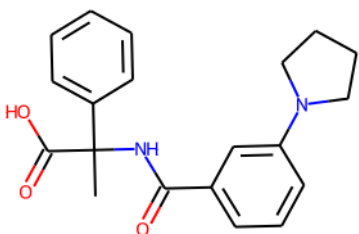
Chemical Structure	SMILES	Vendor
	<chem>N#Cc1cc(C#N)cc(CNc2ccc(CN3CCCC3=O)c2)c1</chem>	ENAMINE Z3860148069
	<chem>CC1(C)CN(C(=O)c2snc(O)c2Cl)c2ccc(Cl)cc21</chem>	ENAMINE PV-002282703459
	<chem>COc1cccc1C1(NC2CC(C)N(C3CC3)C2)CC1</chem>	ENAMINE Z2444182103

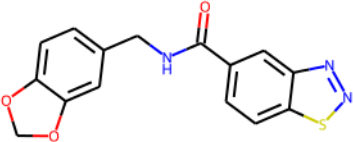
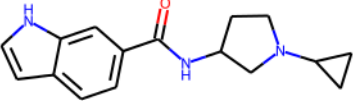
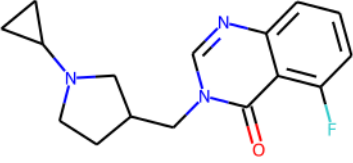
Chemical Structure	SMILES	Vendor
	<chem>CC1CN(C2CC2)CC1NC(=O)CCCCc1c[nH]c2ccccc12</chem>	ENAMINE Z4503477380
	<chem>CCN(CC(=O)NCc1cc(Cl)c(Cl)c(Cl)c1)C1CC1</chem>	ENAMINE Z2086124685
	<chem>CN1CC(N(C)C(=O)c2cc(-n3cccc3)ccn2)C1</chem>	ENAMINE Z4032035979

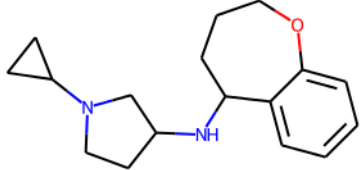
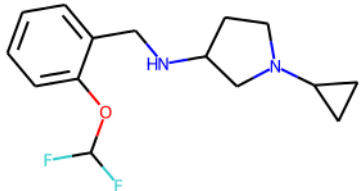
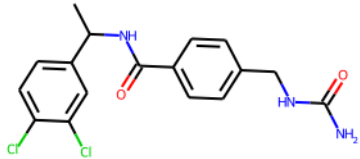
Chemical Structure	SMILES	Vendor
	<chem>O=C(c1ccccc1)N1CCC(CN(C2CC2)C2CC2)C1</chem>	ENAMINE Z2706420680
	<chem>CN1C[C@H]2CN(C(=O)c3cc(Br)c([N+](=O)[O-])[nH]3)C[C@H]2C1</chem>	ENAMINE Z4105653389
	<chem>NC(=O)C1(c2ccccc2)CCN(c2ccc3ccncc3c2)C1</chem>	ENAMINE PV-002991895173

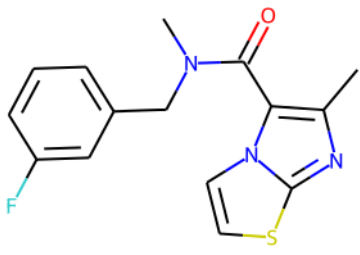
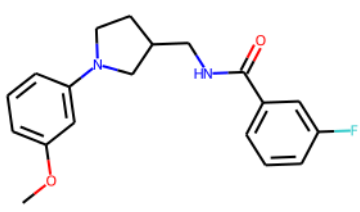
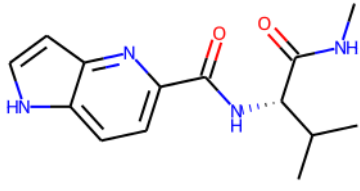
Chemical Structure	SMILES	Vendor
 A chemical structure showing a cyclopentane ring with a nitrogen atom substituted with a cyclopropyl group. The nitrogen is also bonded to a methylene group, which is connected to an amide group (-NH-C(=O)-). The amide group is further connected to a para-chlorophenyl ring.	<chem>O=C(NCC1CCN(C2CC2)C1)c1ccc(Cl)cc1</chem>	MCULE MCULE-8784635667
 A chemical structure featuring a thiazole ring system. The thiazole is connected to a carbonyl group, which is linked to a nitrogen atom. This nitrogen is part of a side chain that includes a propyl group and an ether linkage to a para-ethylphenyl ring.	<chem>CCc1cccc(OCCCN(C)C(=O)c2cn3ccsc3n2)c1</chem>	MCULE MCULE-4581734600
 A chemical structure showing a brominated benzofuran system. The benzofuran is connected to a carbonyl group, which is linked to a nitrogen atom. This nitrogen is part of a side chain that includes a propyl group and a cyclopropyl group.	<chem>CC1CN(C2CC2)CC1NC(=O)c1cc2cc(Br)ccc2o1</chem>	MCULE MCULE-2210026726

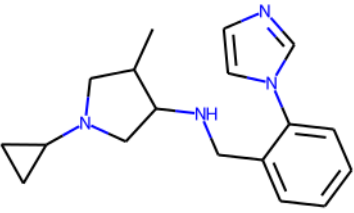
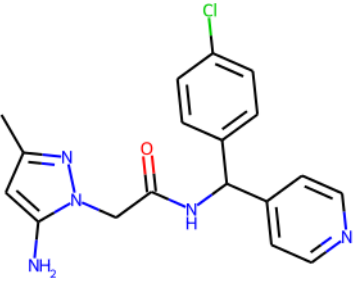
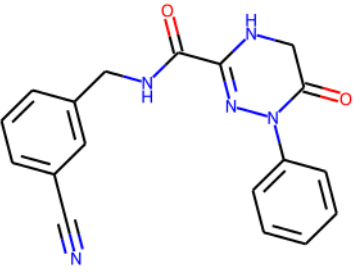
170

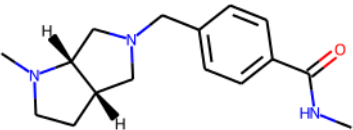
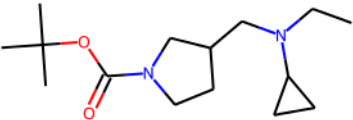
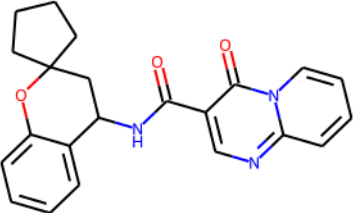
Chemical Structure	SMILES	Vendor
	<chem>Cc1c(C#N)c2ccccc2n1C(=O)N1CCc2ccccc2C1</chem>	MCULE MCULE-3206750891
	<chem>COc1cccc2c1OCCCN(C(=O)c3nc4ccsc4n3)C2</chem>	MCULE MCULE-2909477538
	<chem>CC(NC(=O)c1cccc(N2CC(C2)c1)(C(=O)O)c1ccccc1</chem>	MCULE MCULE-7796909514

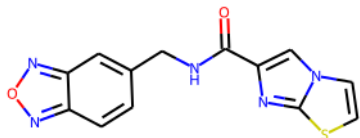
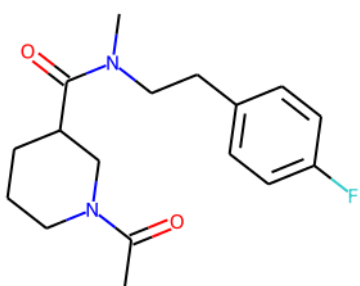
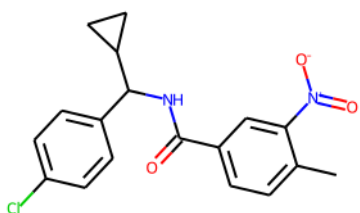
Chemical Structure	SMILES	Vendor
	<chem>O=C(NCc1ccc2c(c1)OCO2)c1ccc2snnc2c1</chem>	MCULE MCULE-3705467470
	<chem>O=C(NC1CCN(C2CC2)C1)c1ccc2cc[nH]c2c1</chem>	MCULE MCULE-2698738093
	<chem>O=c1c2c(F)cccc2ncn1C1CCN(C2CC2)C1</chem>	MCULE MCULE-2340654883

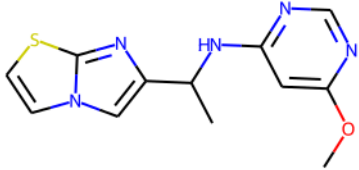
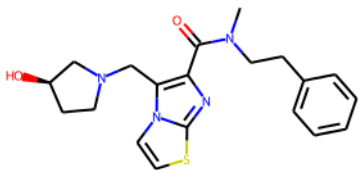
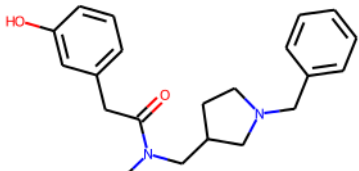
Chemical Structure	SMILES	Vendor
	<chem>c1ccc2c(c1)OCCCC2NC1CCN(C2CC2)C1</chem>	MCULE MCULE-1806993863
	<chem>FC(F)Oc1ccccc1CNC1CCN(C2CC2)C1</chem>	MCULE MCULE-7126639448
	<chem>CC(NC(=O)c1ccc(CNC(N)=O)cc1)c1ccc(Cl)c(Cl)c1</chem>	MCULE MCULE-1695376670

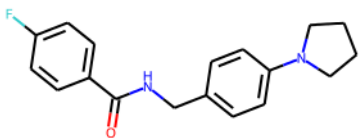
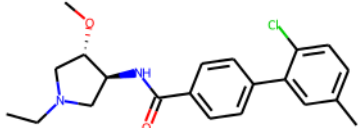
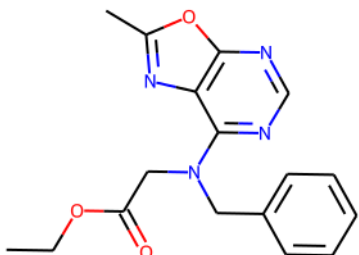
Chemical Structure	SMILES	Vendor
	<chem>Cc1nc2sc[n+]2c1C(=O)N(C)Cc1ccc(F)c1</chem>	MCULE MCULE-2503164160
	<chem>COc1ccc(N2CCC(CNC(=O)c3ccc(F)c3)C2)c1</chem>	MCULE MCULE-1200915253
	<chem>CNC(=O)[C@@H](NC(=O)c1ccc2[nH]ccc2n1)C(C)C</chem>	MCULE MCULE-2506750112

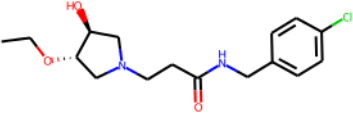
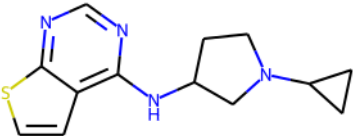
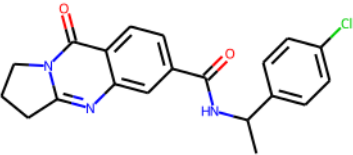
Chemical Structure	SMILES	Vendor
	<chem>CC1CN(C2CC2)CC1NCc1ccccc1-n1ccnc1</chem>	MCULE MCULE-7725475580
	<chem>Cc1cc(N)n(CC(=O)NC(c2ccncc2)c2ccc(Cl)cc2)n1</chem>	MCULE MCULE-4717614306
	<chem>N#Cc1cccc(CNC(=O)C2=NN(c3ccccc3)C(=O)CN2)c1</chem>	MCULE MCULE-5175282400

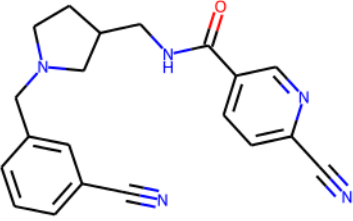
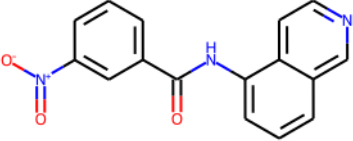
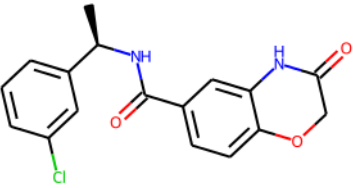
Chemical Structure	SMILES	Vendor
	<chem>CNC(=O)c1ccc(CN2C[C@H]3CCN(C)[C@@H]3C2)cc1</chem>	MCULE MCULE-1518699206
	<chem>CCN(CC1CCN(C(=O)OC(C)(C)C)C1)C1CC1</chem>	MCULE MCULE-9097242731
	<chem>O=C(NC1CC2(CCCC2)Oc2ccccc21)c1cnc2cccn2c1=O</chem>	MCULE MCULE-5391999521


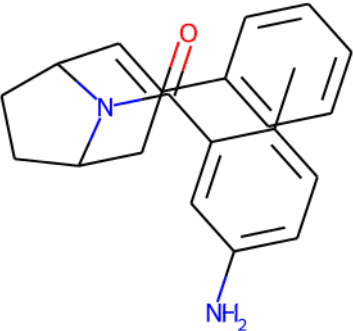
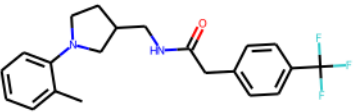
Chemical Structure	SMILES	Vendor
	<chem>O=C(NCc1ccc2nonc2c1)c1cn2ccsc2n1</chem>	MCULE MCULE-8413223026
	<chem>CC(=O)N1CCCC(C(=O)N(C)CCc2ccc(F)cc2)C1</chem>	MCULE MCULE-6488015702
	<chem>Cc1ccc(C(=O)NC(c2ccc(Cl)cc2)C2CC2)cc1[N+](=O)[O-]</chem>	MCULE MCULE-8760425560

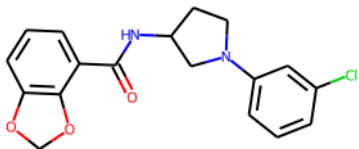
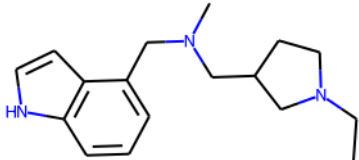
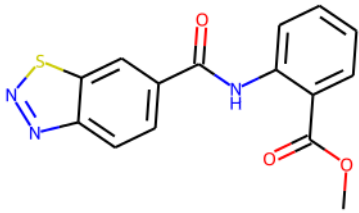
Chemical Structure	SMILES	Vendor
	<chem>COc1cc(NC(C)c2cn3ccsc3n2)ncn1</chem>	MCULE MCULE-3848808801
	<chem>CN(CCc1ccccc1)C(=O)c1nc2scn2c1CN1CC[C@H](O)C1</chem>	MCULE MCULE-5679114822
	<chem>CN(CC1CCN(Cc2ccccc2)C1)C(=O)Cc1cccc(O)c1</chem>	MCULE MCULE-2615922237

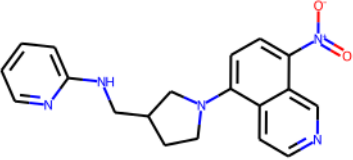
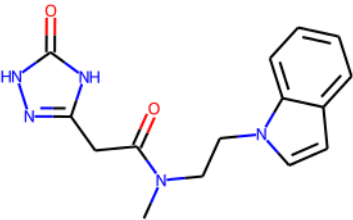
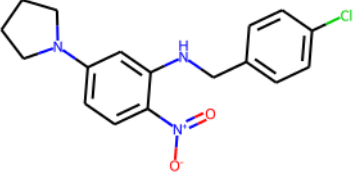
Chemical Structure	SMILES	Vendor
	<chem>O=C(NCc1ccc(N2CCCC2)cc1)c1ccc(F)cc1</chem>	MCULE MCULE-3498450162
	<chem>CCN1C[C@H](NC(=O)c2ccc(-c3cc(C)ccc3Cl)cc2)[C@@H](OC)C1</chem>	MCULE MCULE-8543998375
	<chem>CCOC(=O)CN(Cc1cccc1)c1ncnc2oc(C)nc12</chem>	MCULE MCULE-7529743638

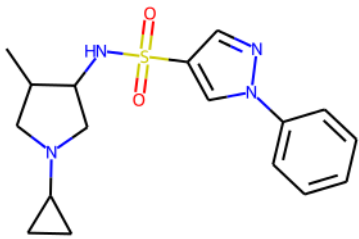
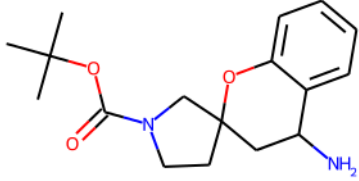
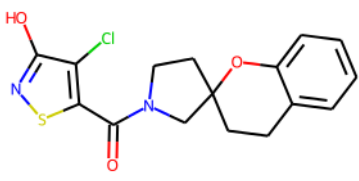
Chemical Structure	SMILES	Vendor
	<chem>CCO[C@H]1CN(CCC(=O)Nc2ccc(Cl)cc2)C[C@H]1O</chem>	MCULE MCULE-7849339301
	<chem>c1nc(NC2CCN(C3CC3)C2)c2ccsc2n1</chem>	MCULE MCULE-3574334271
	<chem>CC(NC(=O)c1ccc2c(=O)n3c(nc2c1)CCC3)c1ccc(Cl)cc1</chem>	MCULE MCULE-8967688073

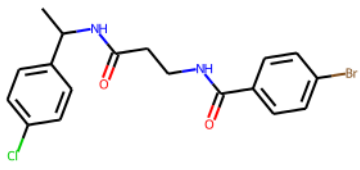
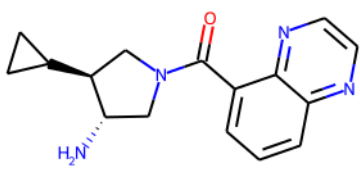
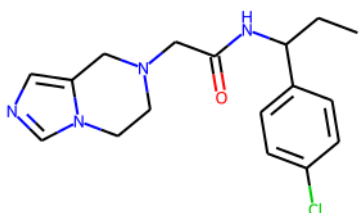
Chemical Structure	SMILES	Vendor
	<chem>N#Cc1cccc(CN2CCC(CNC(=O)c3ccc(C#N)nc3)C2)c1</chem>	MCULE MCULE-4579629250
	<chem>O=C(Nc1cccc2cnccc12)c1cccc([N+](=O)[O-])c1</chem>	MCULE MCULE-8572853695
	<chem>C[C@@H](NC(=O)c1ccc2c(c1)NC(=O)CO2)c1cccc(Cl)c1</chem>	MCULE MCULE-2835383610

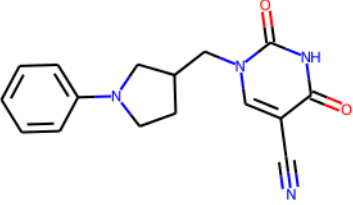
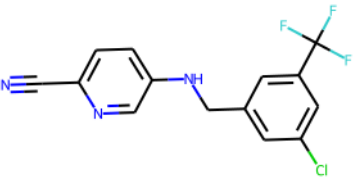
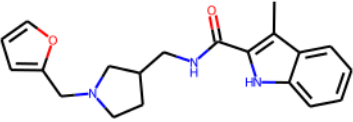
Chemical Structure	SMILES	Vendor
	<chem>O=C(Cc1cn2ccsc2n1)NC1(c2ccc(Cl)cc2)CC1</chem>	MCULE MCULE-3720455446
	<chem>Cc1ccc(N)cc1C(=O)N1C2C=C(c3ccccc3)CC1CC2</chem>	MCULE MCULE-1768739741
	<chem>Cc1ccccc1N1CCC(CNC(=O)Cc2ccc(C(F)(F)F)cc2)C1</chem>	MCULE MCULE-7550173904

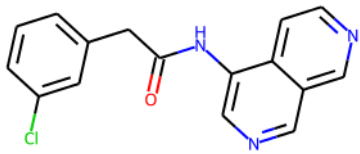
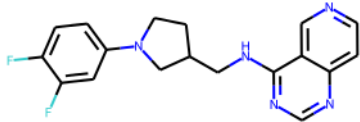
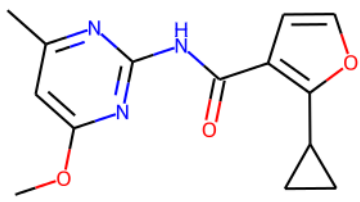
Chemical Structure	SMILES	Vendor
	<chem>O=C(NC1CCN(c2cccc(Cl)c2)C1)c1cccc2c1OCO2</chem>	MCULE MCULE-5430114596
	<chem>CCN1CCC(CN(C)Cc2cccc3[nH]ccc23)C1</chem>	MCULE MCULE-4281557305
	<chem>COC(=O)c1cccc1NC(=O)c1ccc2nnsc2c1</chem>	MCULE MCULE-6091378707

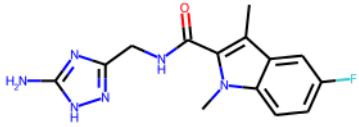
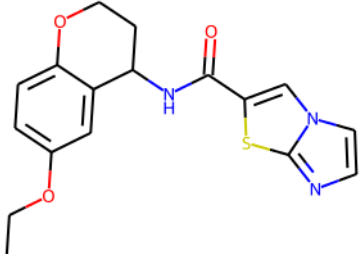
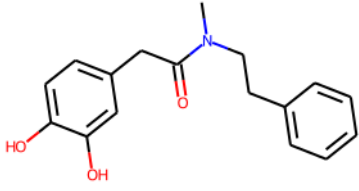
Chemical Structure	SMILES	Vendor
	<chem>O=[N+]([O-])c1ccc(N2CCC(CNc3ccccn3)C2)c2ccncc12</chem>	MCULE MCULE-7480074517
	<chem>CN(CCn1ccc2ccccc21)C(=O)Cc1n[nH]c(=O)[nH]1</chem>	MCULE MCULE-3433129797
	<chem>O=[N+]([O-])c1ccc(N2CCCC2)cc1NCc1ccc(Cl)cc1</chem>	MCULE MCULE-9845865533

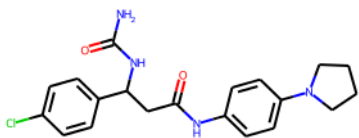
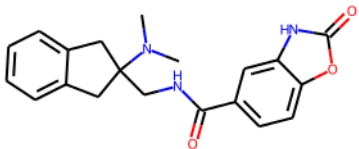
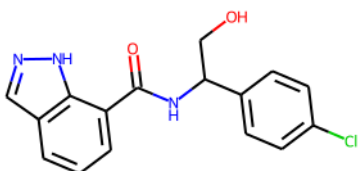
Chemical Structure	SMILES	Vendor
	<chem>CC1CN(C2CC2)CC1NS(=O)(=O)c1cnn(-c2ccccc2)c1</chem>	MCULE MCULE-8737031215
	<chem>CC(C)(C)OC(=O)N1CCC2(CC(N)c3ccccc3O2)C1</chem>	MCULE MCULE-9911953696
	<chem>O=C(c1snc(O)c1Cl)N1C(CC2(CCc3ccccc3O2)C1</chem>	MCULE MCULE-3846136896

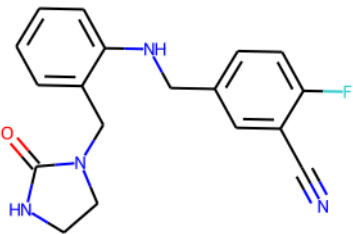
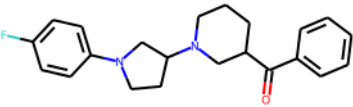
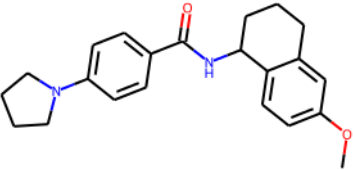
Chemical Structure	SMILES	Vendor
	<chem>CC(NC(=O)CCNC(=O)c1ccc(Br)cc1)c1ccc(Cl)cc1</chem>	MCULE MCULE-7413725165
	<chem>N[C@H]1CN(C(=O)c2ccc3ncnc23)C[C@@H]1C1CC1</chem>	MCULE MCULE-2632711399
	<chem>CCC(NC(=O)CN1CCn2cnc2C1)c1ccc(Cl)cc1</chem>	MCULE MCULE-6699382399

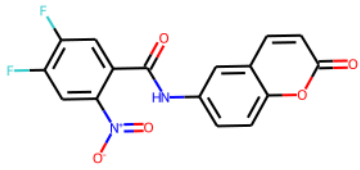
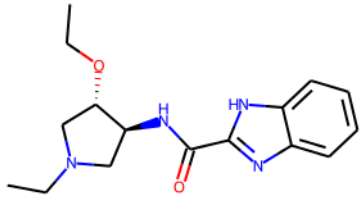
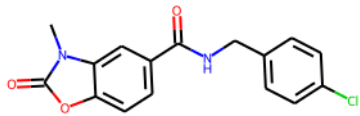
Chemical Structure	SMILES	Vendor
	<chem>N#Cc1cn(CC2CCN(c3ccc cc3)C2)c(=O)[nH]c1=O</chem>	MCULE MCULE-5918466374
	<chem>N#Cc1ccc(NCc2cc(Cl)c c(C(F)(F)F)c2)cn1</chem>	MCULE MCULE-7960935474
	<chem>Cc1c(C(=O)NCC2CCN(Cc 3ccco3)C2)[nH]c2ccccc12</chem>	MCULE MCULE-8221547882

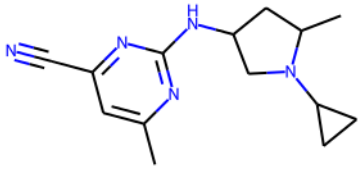
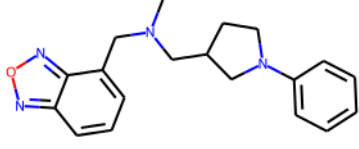
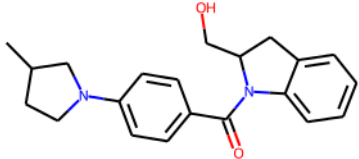
Chemical Structure	SMILES	Vendor
	<chem>O=C(Cc1ccc(Cl)c1)Nc1cncc2cnccc12</chem>	MCULE MCULE-2686285932
	<chem>Fc1ccc(N2CCC(CNc3cncc4cnccc34)C2)cc1F</chem>	MCULE MCULE-1688778845
	<chem>COc1cc(C)nc(NC(=O)c2ccoc2C3CC3)n1</chem>	MCULE MCULE-3482072072

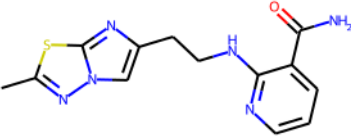
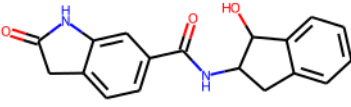
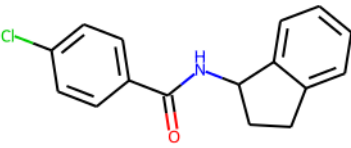
Chemical Structure	SMILES	Vendor
	<chem>Cc1c(C(=O)NCc2n[nH]c(N)n2)n(C)c2ccc(F)cc12</chem>	MCULE MCULE-4316765449
	<chem>CCOc1ccc2c(c1)C(NC(=O)c1cn3ccnc3s1)CCO2</chem>	MCULE MCULE-7660554428
	<chem>CN(CCc1ccccc1)C(=O)Cc1ccc(O)c(O)c1</chem>	MCULE MCULE-6983142451

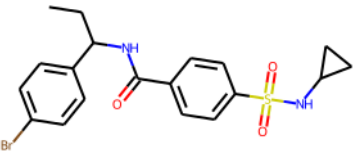
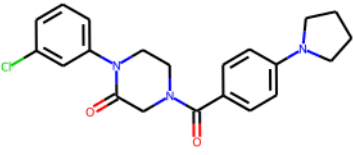
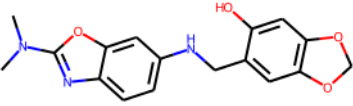
Chemical Structure	SMILES	Vendor
	<chem>NC(=O)NC(CC(=O)Nc1ccc(N2CCCC2)cc1)c1ccc(Cl)cc1</chem>	MCULE MCULE-6269614591
	<chem>CN(C)C1(CNC(=O)c2ccc3oc(=O)[nH]c3cc2)Cc2cccc2C1</chem>	MCULE MCULE-5308302650
	<chem>O=C(NC(CO)c1ccc(Cl)cc1)c1cccc2cn[nH]c12</chem>	MCULE MCULE-8914358363

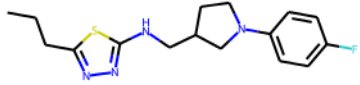
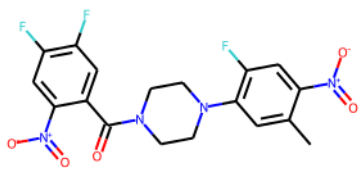
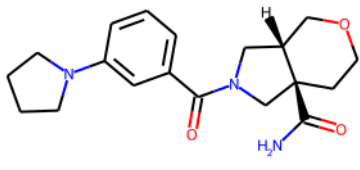
Chemical Structure	SMILES	Vendor
	<chem>N#Cc1cc(CNc2ccccc2CN2CCNC2=O)ccc1F</chem>	MCULE MCULE-6437061504
	<chem>O=C(c1ccccc1)C1CCCN(C2CCN(c3ccc(F)cc3)C2)C1</chem>	MCULE MCULE-5327995555
	<chem>COc1ccc2c(c1)CCCC2NC(=O)c1ccc(N2CCCC2)cc1</chem>	MCULE MCULE-5814210443

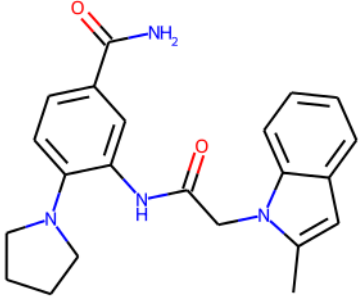
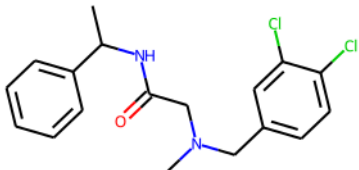
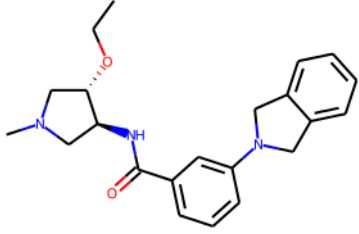
Chemical Structure	SMILES	Vendor
	<chem>O=C(Nc1ccc2oc(=O)ccc2c1)c1cc(F)c(F)cc1[N+](=O)[O-]</chem>	MCULE MCULE-8573286562
	<chem>CCO[C@H]1CN(CC)C[C@@H]1NC(=O)c1nc2ccccc2[nH]1</chem>	MCULE MCULE-3895132333
	<chem>Cn1c(=O)oc2ccc(C(=O)NCc3ccc(Cl)cc3)cc21</chem>	MCULE MCULE-8658028316

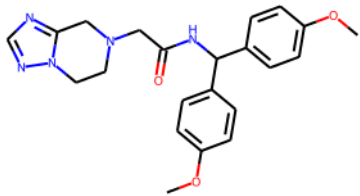
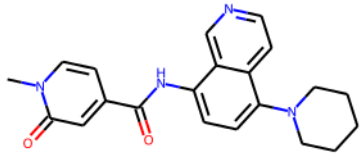
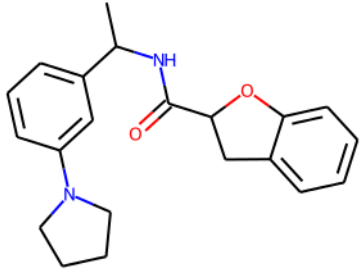
Chemical Structure	SMILES	Vendor
	<chem>Cc1cc(C#N)nc(NC2CC(C)N(C3CC3)C2)n1</chem>	MCULE MCULE-2890245563
	<chem>CN(Cc1cccc2nnc12)CC1CCN(c2ccccc2)C1</chem>	MCULE MCULE-5469523888
	<chem>CC1CCN(c2ccc(C(=O)N3Cc4ccccc4C3CO)cc2)C1</chem>	MCULE MCULE-2577104645

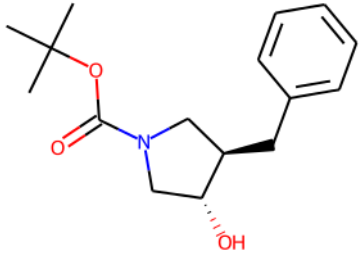
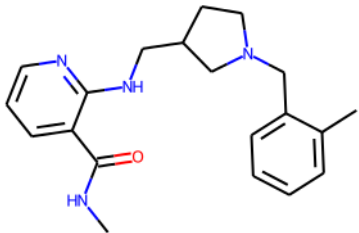
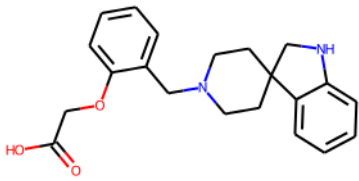
Chemical Structure	SMILES	Vendor
	<chem>Cc1nn2cc(CCNC(=O)c3ccncc3)ncc2s1</chem>	MCULE MCULE-8449512198
	<chem>O=C1Cc2ccc(C(=O)NC3Cc4ccccc4C3O)cc2N1</chem>	MCULE MCULE-7924014972
	<chem>O=C(NC1CCc2ccccc21)c1ccc(Cl)cc1</chem>	MCULE MCULE-6798569132

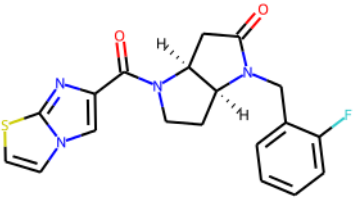
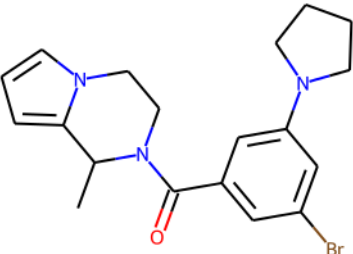
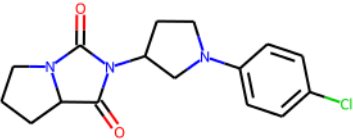
Chemical Structure	SMILES	Vendor
	<chem>CCC(NC(=O)c1ccc(S(=O)(=O)NC2CC2)cc1)c1ccc(Br)cc1</chem>	MCULE MCULE-1206519699
	<chem>O=C(c1ccc(N2CCCC2)cc1)N1CCN(c2cccc(Cl)c2)C(=O)C1</chem>	MCULE MCULE-6992230568
	<chem>CN(C)c1nc2ccc(NCc3cc4c(cc3O)OCO4)cc2o1</chem>	MCULE MCULE-3316839251

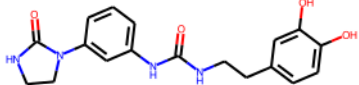
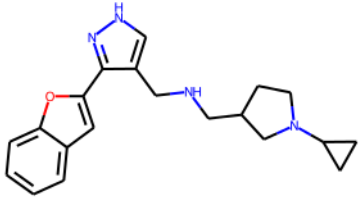
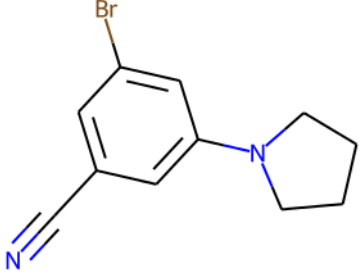
Chemical Structure	SMILES	Vendor
	<chem>CCCC1nnc(NCC2CCN(c3ccc(Cl)cc3)C2)s1</chem>	MCULE MCULE-2737628619
	<chem>Cc1cc(N2CCN(C(=O)c3cc(F)c(F)cc3[N+](=O)[O-])CC2)c(F)cc1[N+](=O)[O-]</chem>	MCULE MCULE-1420653151
	<chem>NC(=O)[C@]12CCOC[C@H]1CN(C(=O)c1cccc(N3CCCC3)c1)C2</chem>	MCULE MCULE-5774735360

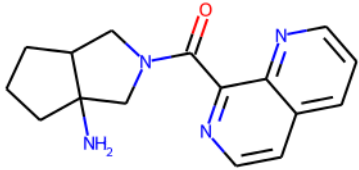
Chemical Structure	SMILES	Vendor
	<chem>Cc1cc2ccccc2n1CC(=O)Nc1cc(C(N)=O)ccc1N1CCCC1</chem>	MCULE MCULE-4493092349
	<chem>CC(NC(=O)CN(C)Cc1ccc(Cl)c(Cl)c1)c1ccccc1</chem>	MCULE MCULE-9765289162
	<chem>CCO[C@H]1CN(C)C[C@@H]1NC(=O)c1ccccc(N2Cc3ccccc3C2)c1</chem>	MCULE MCULE-6186266157

Chemical Structure	SMILES	Vendor
	<chem>COc1ccc(C(=O)NC2C=CC=C2)cc1</chem>	MCULE MCULE-5772008771
	<chem>COc1ccc(C(=O)NC2C=CC=C2)cc1</chem>	MCULE MCULE-4550519519
	<chem>CC(=O)NC1C=CC=C1</chem>	MCULE MCULE-5452602371

Chemical Structure	SMILES	Vendor
	<chem>CC(C)(C)OC(=O)N1C[C@H](O)[C@H](Cc2ccccc2)C1</chem>	MCULE MCULE-7598963182
	<chem>CNC(=O)c1cccnc1NCC1C CN(Cc2ccccc2C)C1</chem>	MCULE MCULE-1272677437
	<chem>O=C(O)COc1ccccc1CN1C CC2(CC1)CNc1ccccc12</chem>	MCULE MCULE-1515243721

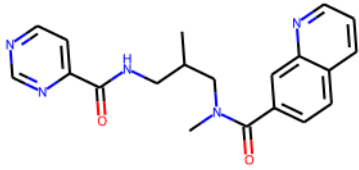
Chemical Structure	SMILES	Vendor
	<chem>O=C1C[C@H]2[C@H](CCN2C(=O)c2cn3ccsc3n2)N1Cc1ccccc1F</chem>	MCULE MCULE-7374409985
	<chem>CC1c2cccn2CCN1C(=O)c1cc(Br)cc(N2CCCC2)c1</chem>	MCULE MCULE-2789596719
	<chem>O=C1C2CCCN2C(=O)N1C1CCN(c2ccc(Cl)cc2)C1</chem>	MCULE MCULE-4207112797

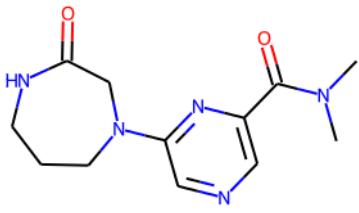
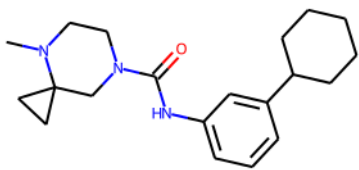
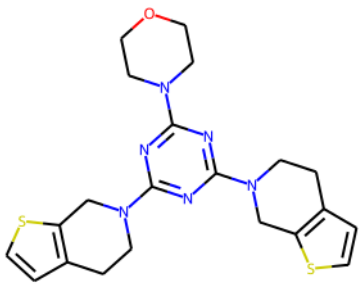
Chemical Structure	SMILES	Vendor
	<chem>O=C(NCCc1ccc(O)c(O)c1)Nc1cccc(N2CCNC2=O)c1</chem>	MCULE MCULE-4999491482
	<chem>c1ccc2oc(-c3n[nH]cc3)cc2c1</chem> <chem>CNCC3CCN(C4CC4)C3)cc2c1</chem>	MCULE MCULE-6824182077
	<chem>N#Cc1cc(Br)cc(N2CCCC2)c1</chem>	MCULE MCULE-7191624798

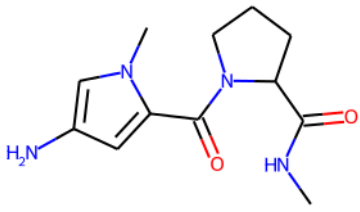
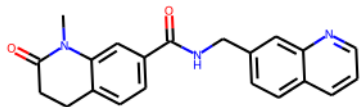
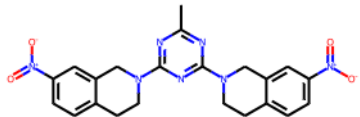
Chemical Structure	SMILES	Vendor
	<chem>NC12CCCC1CN(C(=O)c1nccc3ccncc13)C2</chem>	MCULE MCULE-8359482340

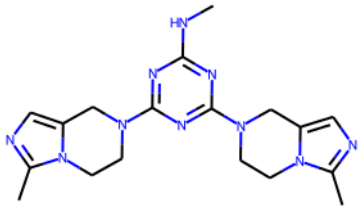
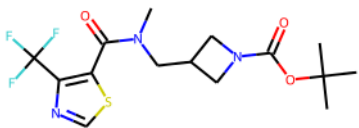
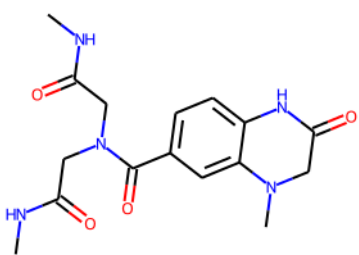
4 RFWD3

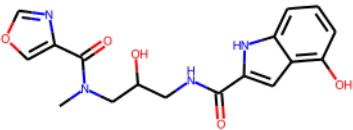
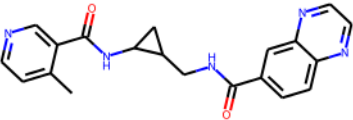
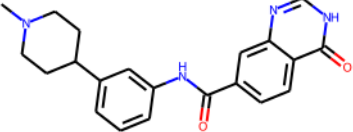
UniProtKB entry Q6PCD5

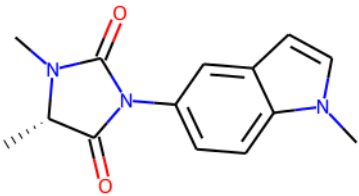
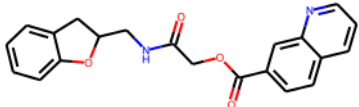
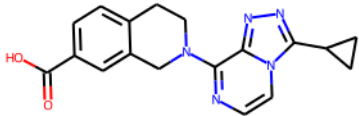
Chemical Structure	SMILES	Vendor
	<chem>CC(CNC(=O)c1ccncc1)C(=O)c1ccc2ccncc2c1</chem>	ENAMINE PV-004042153556

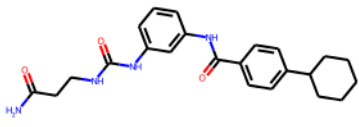
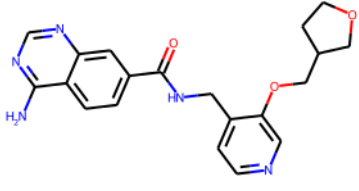
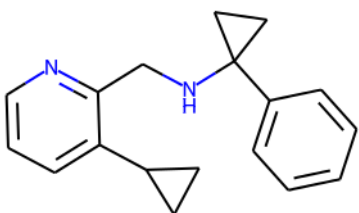
Chemical Structure	SMILES	Vendor
	<chem>CN(C)C(=O)c1cncc(N2C CCNC(=O)C2)n1</chem>	ENAMINE Z2090545450
	<chem>CN1CCN(C(=O)Nc2cccc(C3CCCCC3)c2)CC12CC2</chem>	ENAMINE PV-003001277413
	<chem>c1cc2c(s1)CN(c1nc(N3 CCOCC3)nc(N3CCc4ccsc4C3)n1)CC2</chem>	ENAMINE Z1554709366

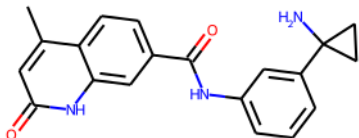
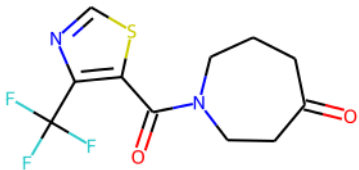
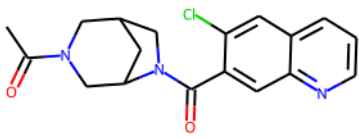
Chemical Structure	SMILES	Vendor
	<chem>CNC(=O)C1CCCN1C(=O)c1cc(N)cn1C</chem>	ENAMINE Z3228632917
	<chem>CN1C(=O)CCc2ccc(C(=O)NCc3ccc4ccnnc4c3)cc21</chem>	ENAMINE PV-002131520859
	<chem>Cc1nc(N2CCc3ccc([N+](=O)[O-])cc3C2)nc(N2CCc3ccc([N+](=O)[O-])cc3C2)n1</chem>	ENAMINE Z1731165093

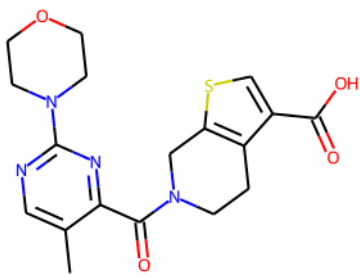
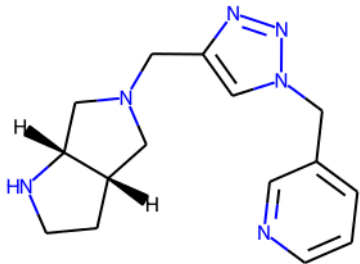
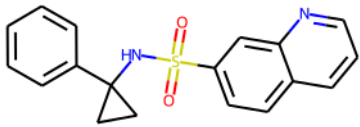
Chemical Structure	SMILES	Vendor
	<chem>CNc1nc(N2CCn3c(cnc3C)C2)nc(N2CCn3c(cnc3C)C2)n1</chem>	ENAMINE Z3078723506
	<chem>CN(CC1CN(C(=O)OC(C)(C)C)C1)C(=O)c1scnc1C(F)(F)F</chem>	ENAMINE Z3702164053
	<chem>CNC(=O)CN(CC(=O)NC)C(=O)c1ccc2c(c1)N(C)CC(=O)N2</chem>	ENAMINE PV-003718129906

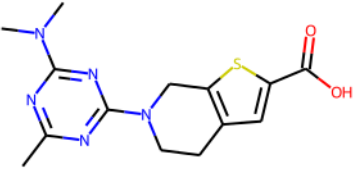
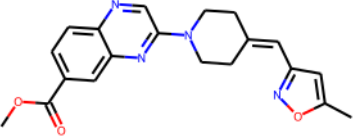
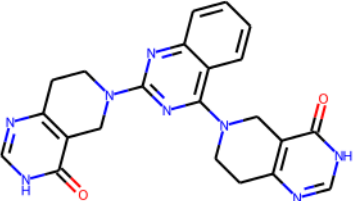
Chemical Structure	SMILES	Vendor
	<chem>CN(CC(O)CNC(=O)c1cc2c(O)cccc2[nH]1)C(=O)c1cncn1</chem>	ENAMINE PV-003365144759
	<chem>Cc1ccncc1C(=O)NC1CC1CNC(=O)c1ccc2ncncn2c1</chem>	ENAMINE PV-004011937962
	<chem>CN1CCC(c2cccc(NC(=O)c3ccc4c(=O)[nH]cnc4c3)c2)CC1</chem>	ENAMINE Z3627736825

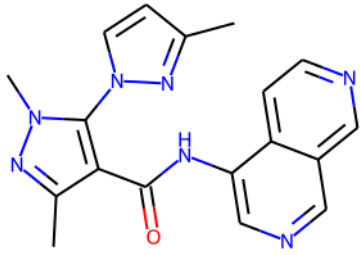

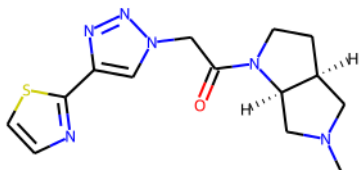
Chemical Structure	SMILES	Vendor
	<chem>C[C@H]1C(=O)N(c2ccc3c(ccn3C)c2)C(=O)N1C</chem>	ENAMINE Z3499889533
	<chem>O=C(COC(=O)c1ccc2cccnc2c1)NCC1Cc2ccccc2O1</chem>	ENAMINE PV-004050168243
	<chem>O=C(O)c1ccc2c(c1)CN(c1nccn3c(C4CC4)nnc13)CC2</chem>	ENAMINE Z2466040826

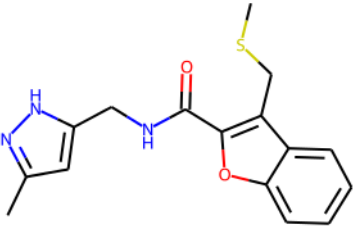
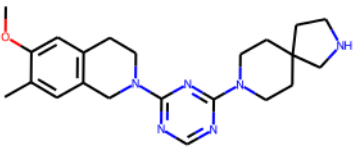
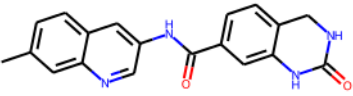
Chemical Structure	SMILES	Vendor
	<chem>NC(=O)CCNC(=O)Nc1ccc c(NC(=O)c2ccc(C3CCCCC3)cc2)c1</chem>	ENAMINE Z1975323972
	<chem>Nc1ncnc2cc(C(=O)NCc3 ccncc3OCC3CCOC3)ccc12</chem>	ENAMINE Z2639482570
	<chem>c1ccc(C2(NCc3ncccc3C3CC3)CC2)cc1</chem>	ENAMINE Z4400876939

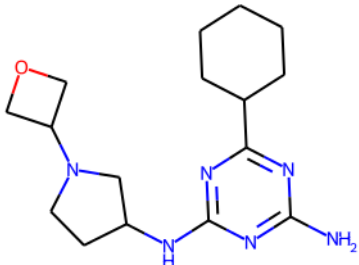
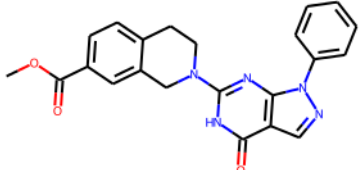
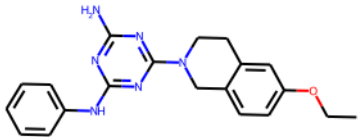
Chemical Structure	SMILES	Vendor
	<chem>Cc1cc(=O)[nH]c2cc(C(=O)Nc3cccc(C4(N)CC4)c3)ccc12</chem>	ENAMINE PV-002754809164
	<chem>O=C1CCCN(C(=O)c2scnc2C(F)(F)F)CC1</chem>	ENAMINE Z3633080745
	<chem>CC(=O)N1CC2CC(C1)N(C(=O)c3cc3ncccc3cc1Cl)C2</chem>	ENAMINE PV-003187176817

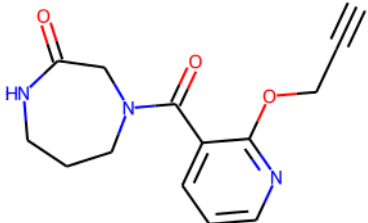
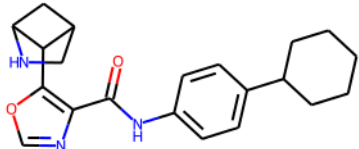
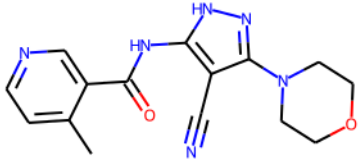
Chemical Structure	SMILES	Vendor
	<chem>Cc1cnc(N2CCOCC2)nc1C(=O)N1CCc2c(C(=O)O)csc2C1</chem>	ENAMINE Z4573419466
	<chem>c1cncc(Cn2cc(CN3C[C@@H]4CCN[C@@H]4C3)nn2)c1</chem>	ENAMINE Z4386977857
	<chem>O=S(=O)(NC1(c2ccccc2)CC1)c1ccc2cccnc2c1</chem>	ENAMINE PV-002737732648

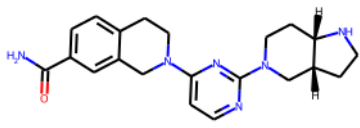
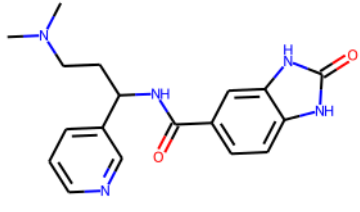
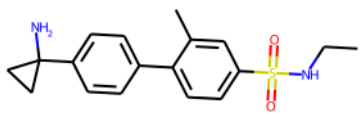
Chemical Structure	SMILES	Vendor
	<chem>Cc1nc(N(C)C)nc(N2CCc3cc(C(=O)O)sc3C2)n1</chem>	ENAMINE Z3346239392
	<chem>COC(=O)c1ccc2ncc(N3C4C(=Cc4cc(C)on4)CC3)nc2c1</chem>	ENAMINE Z3076421991
	<chem>O=c1[nH]cnc2c1CN(c1nc(N3CCc4nc[nH]c(=O)c4C3)c3ccccc3n1)CC2</chem>	ENAMINE Z1494797249

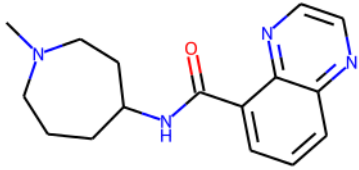
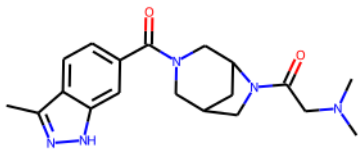
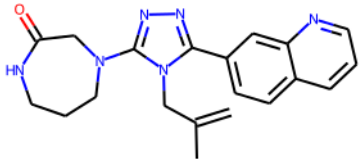
Chemical Structure	SMILES	Vendor
	<chem>Cc1ccn(-c2c(C(=O)Nc3cnc4cnccc34)c(C)nn2C)n1</chem>	ENAMINE PV-003849851985
	<chem>CN(C(=O)C1CC1(F)c1ccc1)C1(c2cccnc2)CC1</chem>	ENAMINE Z4253808924
	<chem>CN1C[C@@H]2CCN(C(=O)Cn3cc(-c4nccs4)nn3)[C@@H]2C1</chem>	ENAMINE PV-003318193975

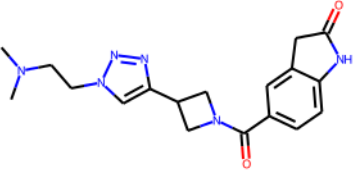
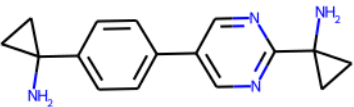
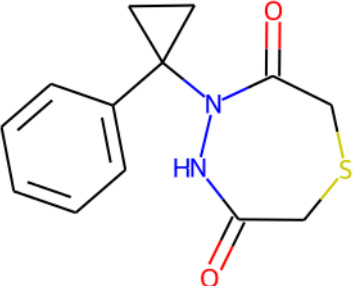
Chemical Structure	SMILES	Vendor
	<chem>CSCc1c(C(=O)NCc2cc(C)n[nH]2)oc2ccccc12</chem>	ENAMINE Z1193209375
	<chem>COc1cc2c(cc1C)CN(c1ncnc(N3CCCC4(CCNC4)CC3)n1)CC2</chem>	ENAMINE Z4080947217
	<chem>Cc1ccc2cc(NC(=O)c3cc4c(c3)NC(=O)NC4)cnc2c1</chem>	ENAMINE PV-002749493459

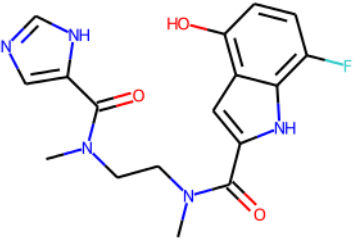
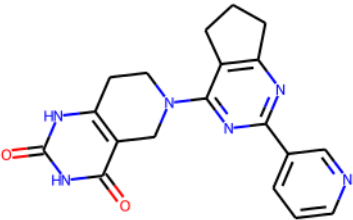
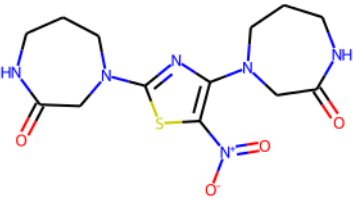
Chemical Structure	SMILES	Vendor
	<chem>Nc1nc(NC2CCN(C3COC3)C2)nc(C2CCCCC2)n1</chem>	ENAMINE Z4232835768
	<chem>COC(=O)c1ccc2c(c1)CN(c1nc3c(cnn3-c3ccccc3)c(=O)[nH]1)CC2</chem>	ENAMINE Z1577016763
	<chem>CCOc1ccc2c(c1)CCN(c1nc(N)nc(Nc3ccccc3)n1)C2</chem>	ENAMINE PV-002507591107

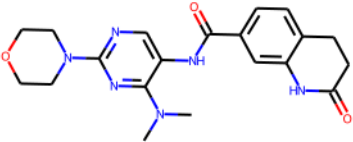
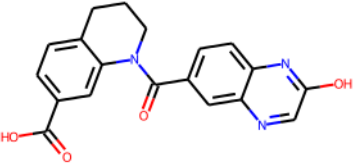
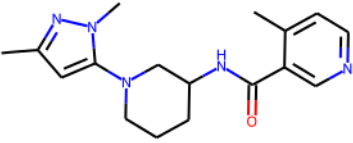
Chemical Structure	SMILES	Vendor
	<chem>C#CCOc1ncccc1C(=O)N1CCCC(=O)C1</chem>	ENAMINE Z1144674871
	<chem>O=C(Nc1ccc(C2CCCCC2)cc1)c1ncoc1C1C2CNC1C2</chem>	ENAMINE PV-003771912644
	<chem>Cc1ccncc1C(=O)Nc1[nH]nc(C#N)c1N2CCOCC2</chem>	ENAMINE PV-002222827088

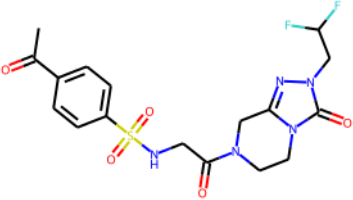

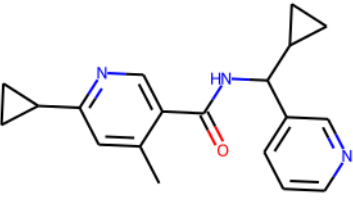
Chemical Structure	SMILES	Vendor
	<chem>NC(=O)c1ccc2c(c1)CN(c1ccnc(N3CC[C@@H]4NC[C@@H]4C3)n1)CC2</chem>	ENAMINE Z4212039022
	<chem>CN(C)CCC(NC(=O)c1ccc2[nH]c(=O)[nH]c2c1)c1ccnc1</chem>	ENAMINE Z2932805635
	<chem>CCNS(=O)(=O)c1ccc(-c2ccc(C3(N)CC3)cc2)c(C)c1</chem>	ENAMINE Z4154046176

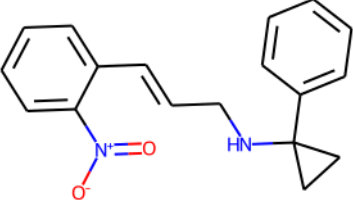
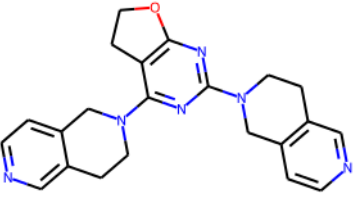
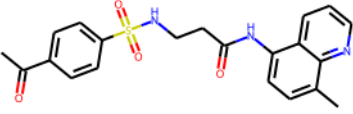
Chemical Structure	SMILES	Vendor
	<chem>CN1CCCC(NC(=O)c2cccc3ncnc23)CC1</chem>	ENAMINE Z4035660196
	<chem>Cc1n[nH]c2cc(C(=O)N3CC4CC(C3)N(C(=O)CN(C)C)C4)ccc12</chem>	ENAMINE PV-003309218792
	<chem>C=C(C)Cn1c(-c2ccc3ccnnc3c2)nnc1N1CCCNC(=O)C1</chem>	ENAMINE Z3144082858

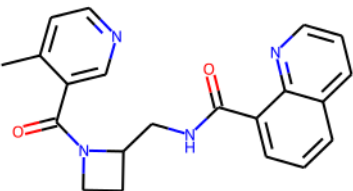
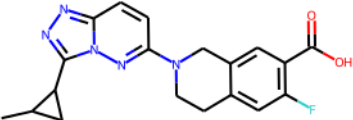
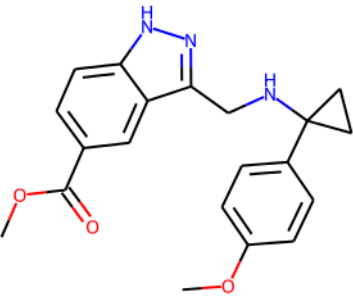
Chemical Structure	SMILES	Vendor
	<chem>CN(C)CCn1cc(C2CN(C(=O)c3ccc4c(c3)CC(=O)N4)C2)nn1</chem>	ENAMINE PV-003505330506
	<chem>NC1(c2ccc(-c3cnc(C4(N)CC4)nc3)cc2)CC1</chem>	ENAMINE Z3547458316
	<chem>O=C1CSCC(=O)N(C2(c3ccccc3)CC2)N1</chem>	ENAMINE Z3827858012

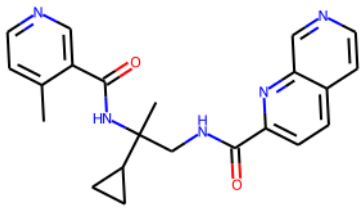
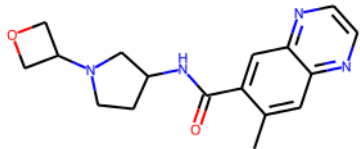
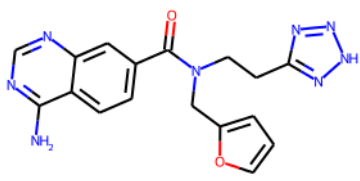
Chemical Structure	SMILES	Vendor
	<chem>CN(CCN(C)C(=O)c1cc2c(O)ccc(F)c2[nH]1)C(=O)c1cnc[nH]1</chem>	ENAMINE PV-003701287247
	<chem>O=c1[nH]c2c(c(=O)[nH]1)CN(c1nc(-c3ccnc3)nc3c1CCC3)CC2</chem>	ENAMINE PV-004022616597
	<chem>O=C1CN(c2nc(N3CCCNC(=O)C3)c([N+](=O)[O-])s2)CCCN1</chem>	ENAMINE Z1225459684

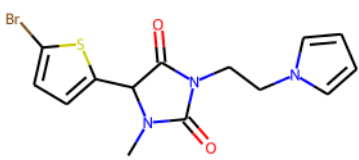
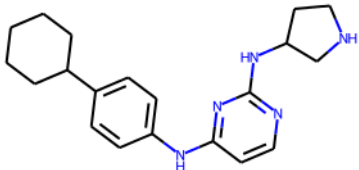
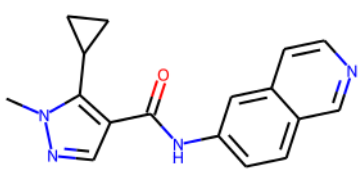
Chemical Structure	SMILES	Vendor
	<chem>CN(C)c1nc(N2CCOCC2)ncc1NC(=O)c1ccc2c(c1)NC(=O)CC2</chem>	ENAMINE Z4250956608
	<chem>O=C(O)c1ccc2c(c1)N(C(=O)c1ccc3nc(O)cnc3c1)CCC2</chem>	ENAMINE PV-003560784201
	<chem>Cc1cc(N2CCCC(NC(=O)c3cnc(C)cc3)C2)n(C)n1</chem>	ENAMINE Z1883088541

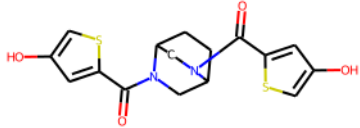
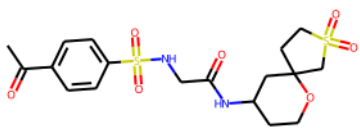
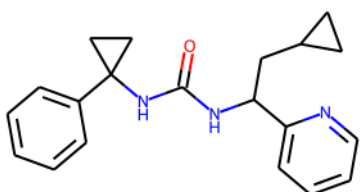
Chemical Structure	SMILES	Vendor
	<chem>CC(=O)c1ccc(S(=O)(=O)NCC(=O)N2CCn3c(nn(C(F)F)c3=O)C2)cc1</chem>	ENAMINE Z1933925060
	<chem>NC(=O)Nc1ccc(NC(=O)c2cc(C3CCCCC3)ccc2O)cc1</chem>	ENAMINE PV-003484996014
	<chem>Cc1cc(C2CC2)ncc1C(=O)NC(c1cccn1)C1CC1</chem>	ENAMINE Z3083147377

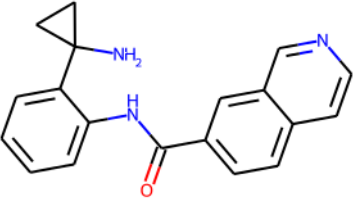
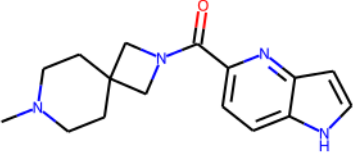
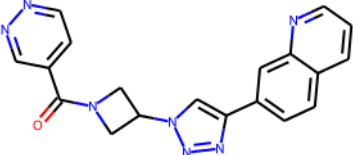
Chemical Structure	SMILES	Vendor
	<chem>O=[N+](O-)[c1ccccc1]C=CCNC1(c2ccccc2)CC1</chem>	ENAMINE Z1168450179
	<chem>c1cc2c(cn1)CCN(c1nc3c(c(c(N4CCc5cnccc5C4)n1)CCO3)C2</chem>	ENAMINE Z4641705334
	<chem>CC(=O)c1ccc(S(=O)(=O)NCCC(=O)Nc2ccc(C)c3ncccc23)cc1</chem>	ENAMINE Z284862138

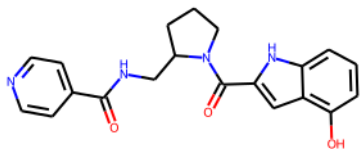
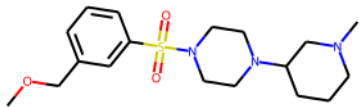
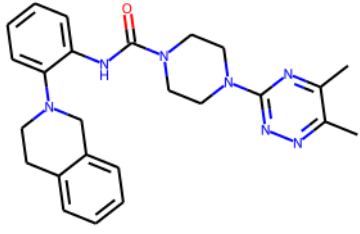
Chemical Structure	SMILES	Vendor
	<chem>Cc1ccncc1C(=O)N1CCC1CNC(=O)c1cccc2cccn12</chem>	ENAMINE PV-000535104446
	<chem>CC1CC1c1nnc2ccc(N3CCc4cc(F)c(C(=O)O)cc4C3)nn12</chem>	ENAMINE Z3346246766
	<chem>COC(=O)c1ccc2[nH]nc(CNC3(c4ccc(OC)cc4)CC3)c2c1</chem>	ENAMINE Z4195181017

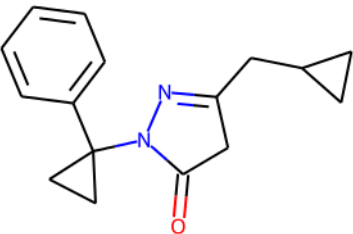
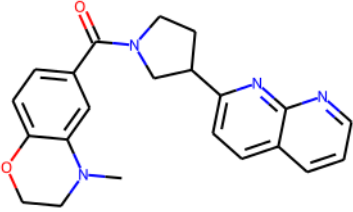
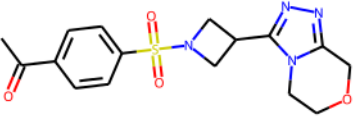
Chemical Structure	SMILES	Vendor
	<chem>Cc1ccncc1C(=O)NC(C)(CNC(=O)c1ccc2ccncc2n1)C1CC1</chem>	ENAMINE Z3726663633
	<chem>Cc1cc2ncnc2cc1C(=O)NC1CCN(C2COC2)C1</chem>	ENAMINE Z4228387019
	<chem>Nc1ncnc2cc(C(=O)N(CCc3nn[nH]n3)Cc3ccco3)ccc12</chem>	ENAMINE PV-003942699351

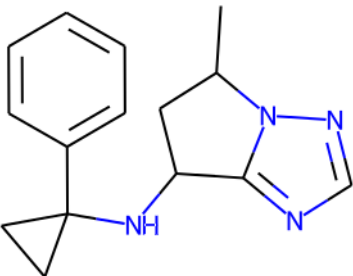
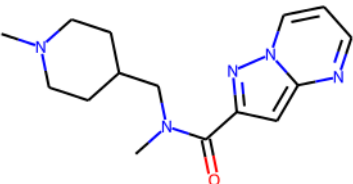
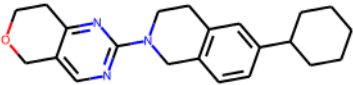
Chemical Structure	SMILES	Vendor
	<chem>CN1C(=O)N(CCn2cccc2)C(=O)C1c1ccc(Br)s1</chem>	ENAMINE Z2769009130
	<chem>c1cc(Nc2ccc(C3CCCCC3)cc2)nc(NC2CCNC2)n1</chem>	ENAMINE PV-003667919713
	<chem>Cn1ncc(C(=O)Nc2ccc3cncnc3c2)c1C1CC1</chem>	ENAMINE PV-002269123650

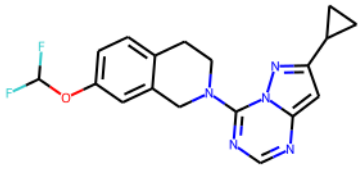
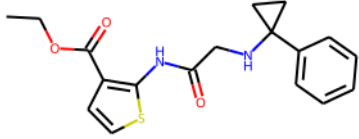
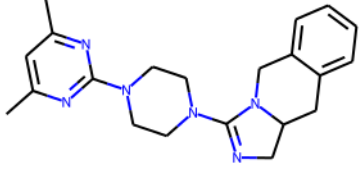
Chemical Structure	SMILES	Vendor
	<chem>O=C(c1cc(O)cs1)N1CC2CCC1CN2C(=O)c1cc(O)cs1</chem>	ENAMINE Z2911223581
	<chem>CC(=O)c1ccc(S(=O)(=O)NCC(=O)NC2CCOC3(CCS(=O)(=O)C3)C2)cc1</chem>	ENAMINE Z1600821985
	<chem>O=C(NC(CC1CC1)c1ccccc1)NC1(CCC1)CC1</chem>	ENAMINE Z3552977111

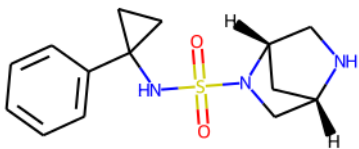
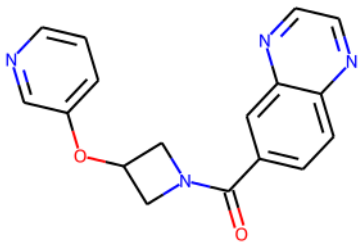
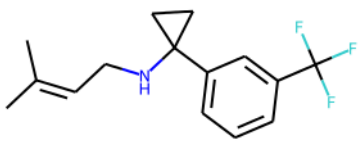
Chemical Structure	SMILES	Vendor
	<chem>NC1(c2ccccc2NC(=O)c2ccc3ccncc3c2)CC1</chem>	ENAMINE PV-003162559744
	<chem>CN1CCC2(CC1)CN(C(=O)c1ccc3[nH]ccc3n1)C2</chem>	ENAMINE Z3589577949
	<chem>O=C(c1ccnnc1)N1CC(n2cc(-c3ccc4ccncc4c3)nn2)C1</chem>	ENAMINE PV-003123496338

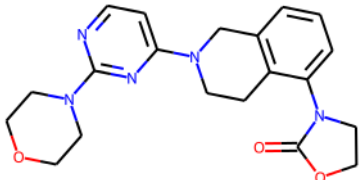
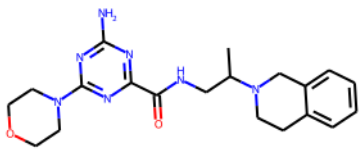
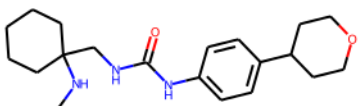
Chemical Structure	SMILES	Vendor
	<chem>O=C(NCC1CCCN1C(=O)c1cc2c(O)cccc2[nH]1)c1ccncc1</chem>	ENAMINE PV-004061740627
	<chem>COCc1cccc(S(=O)(=O)N2CCN(C3CCCN(C)C3)CC2)c1</chem>	ENAMINE Z1212960833
	<chem>Cc1nnc(N2CCN(C(=O)Nc3cccc3N3CCc4cccc4C3)CC2)nc1C</chem>	ENAMINE Z1772032406

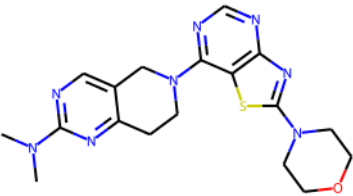
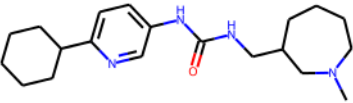
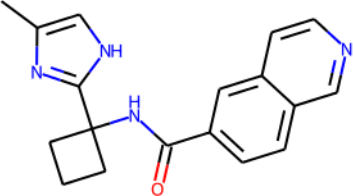
Chemical Structure	SMILES	Vendor
	<chem>O=C1CC(CC2CC2)=NN1C1(c2ccccc2)CC1</chem>	ENAMINE Z3827857738
	<chem>CN1CCOc2ccc(C(=O)N3C(Cc4ccc5ccnnc5n4)C3)cc21</chem>	ENAMINE Z2882573215
	<chem>CC(=O)c1ccc(S(=O)(=O)N2CC(c3nnc4n3CCOC4)C2)cc1</chem>	ENAMINE Z4393404147

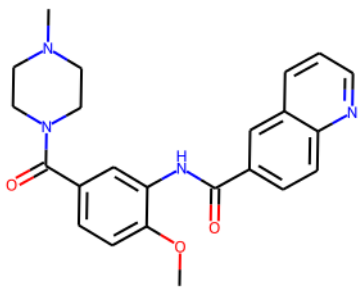
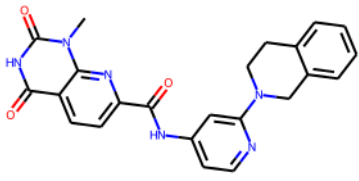
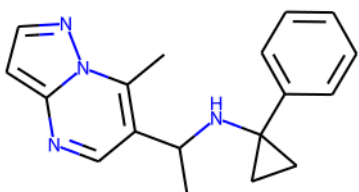
Chemical Structure	SMILES	Vendor
	<chem>CC1CC(NC2(c3ccccc3)CC2)c2ncnn21</chem>	ENAMINE Z2927063148
	<chem>CN1CCC(CN(C)C(=O)c2c3nccccn3n2)CC1</chem>	ENAMINE Z2767624763
	<chem>c1cc2c(cc1C1CCCCC1)C CN(c1ncc3c(n1)CCOC3)C2</chem>	ENAMINE PV-003474556216

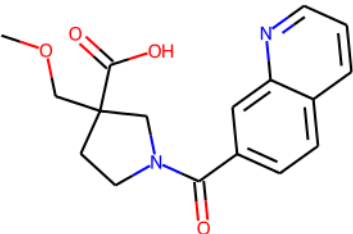
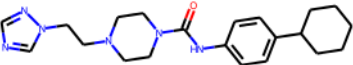
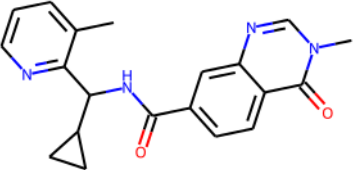
Chemical Structure	SMILES	Vendor
	<chem>FC(F)Oc1ccc2c(c1)CN(c1ncnc3cc(C4CC4)nn13)CC2</chem>	ENAMINE Z3828474263
	<chem>CCOC(=O)c1ccsc1NC(=O)CNC1(c2ccccc2)CC1</chem>	ENAMINE Z1098842328
	<chem>Cc1cc(C)nc(N2CCN(C3=NCC4Cc5ccccc5CN34)CC2)n1</chem>	ENAMINE PV-004018887443

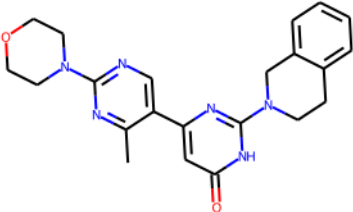
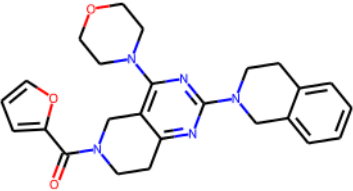
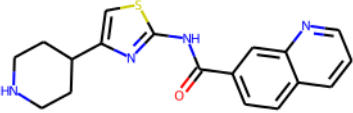
Chemical Structure	SMILES	Vendor
	<chem>O=S(=O)(NC1(c2ccccc2)CC1)N1C[C@H]2C[C@H]1CN2</chem>	ENAMINE Z3365096657
	<chem>O=C(c1ccc2ncnc2c1)N1CC(Oc2cccn2)C1</chem>	ENAMINE Z3244543843
	<chem>CC(C)=CCNC1(c2ccccc2C(F)(F)F)CC1</chem>	ENAMINE Z1098848278

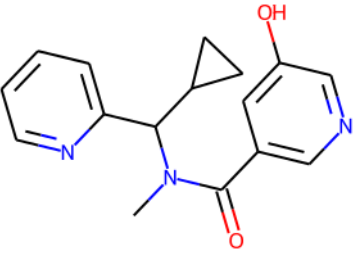
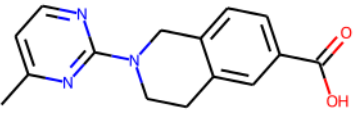
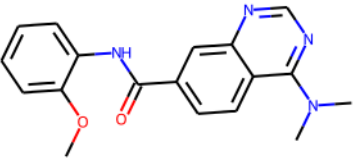
Chemical Structure	SMILES	Vendor
	<chem>O=C1OCCN1c1cccc2c1CCN(c1ccnc(N3CCOCC3)n1)C2</chem>	ENAMINE Z1675285823
	<chem>CC(CNC(=O)c1nc(N)nc(N2CCOCC2)n1)N1CCc2ccccc2C1</chem>	ENAMINE Z2228919240
	<chem>CNC1(CNC(=O)Nc2ccc(C3CCOCC3)cc2)CCCC1</chem>	ENAMINE Z4275499941

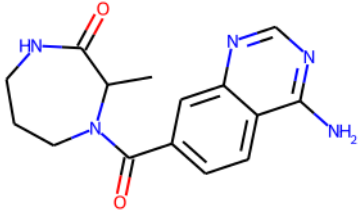
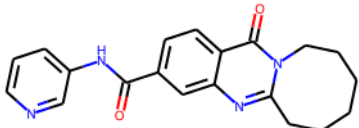
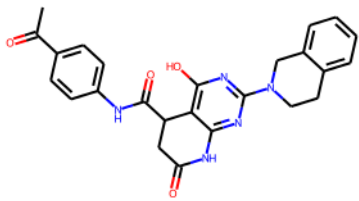
Chemical Structure	SMILES	Vendor
	<chem>CN(C)c1ncc2c(n1)CCN(c1ncnc3nc(N4CCOCC4)sc13)C2</chem>	ENAMINE Z3830276208
	<chem>CN1CCCCC(CNC(=O)Nc2cnc(C3CCCCC3)nc2)C1</chem>	ENAMINE PV-003029680285
	<chem>Cc1c[nH]c(C2(NC(=O)c3ccc4cnccc4c3)CCC2)n1</chem>	ENAMINE Z3363443295

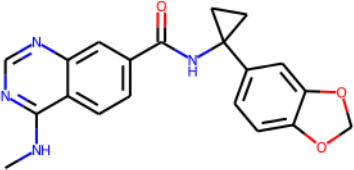
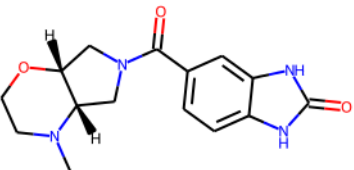
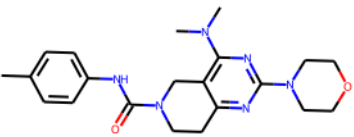
Chemical Structure	SMILES	Vendor
	<chem>COc1ccc(C(=O)N2CCN(CC2)CC2)cc1NC(=O)c1ccc2ncccc2c1</chem>	ENAMINE Z970696414
	<chem>Cn1c(=O)[nH]c(=O)c2ccc(C(=O)Nc3ccnc(N4CCc5ccccc5C4)c3)nc21</chem>	ENAMINE Z2228594727
	<chem>Cc1c(C(C)NC2(c3ccccc3)CC2)cnc2ccnn12</chem>	ENAMINE Z1608121107

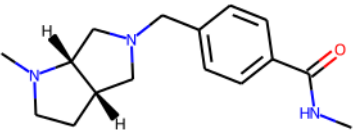
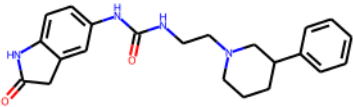
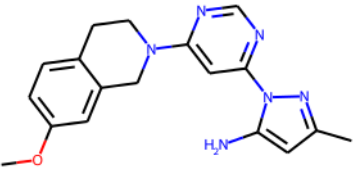
Chemical Structure	SMILES	Vendor
	<chem>COCC1(C(=O)O)CCN(C(=O)c2ccc3cccnc3c2)C1</chem>	MCULE MCULE-4946294935
	<chem>O=C(Nc1ccc(C2CCCCC2)cc1)N1CCN(CCn2cncn2)CC1</chem>	MCULE MCULE-9747378681
	<chem>Cc1ccnc1C(NC(=O)c1ccc2c(=O)n(C)cnc2c1)C1CC1</chem>	MCULE MCULE-4293277751

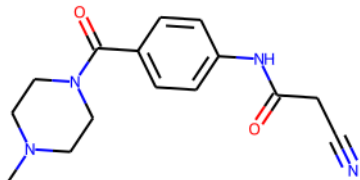
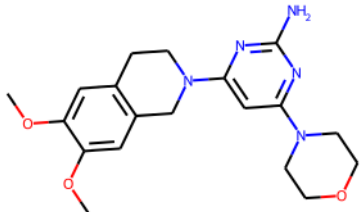
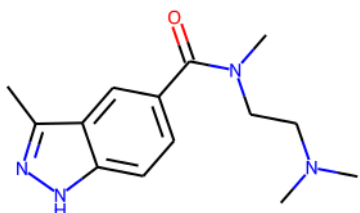
Chemical Structure	SMILES	Vendor
	<chem>Cc1nc(N2CCOCC2)ncc1-c1cc(=O)[nH]c(N2CCc3ccccc3C2)n1</chem>	MCULE MCULE-3380326951
	<chem>O=C(c1ccco1)N1CCc2nc(N3CCc4ccccc4C3)nc(N3CCOCC3)c2C1</chem>	MCULE MCULE-3379448241
	<chem>O=C(Nc1nc(C2CCNCC2)cs1)c1ccc2cccn2c1</chem>	MCULE MCULE-3409920075

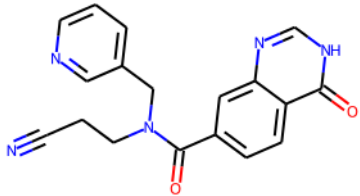
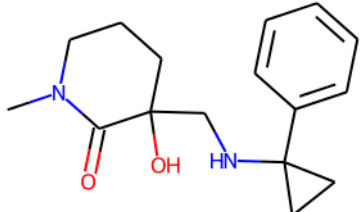
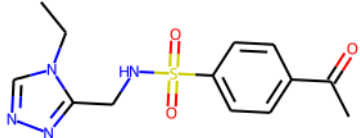
Chemical Structure	SMILES	Vendor
	<chem>CN(C(=O)c1cncc(O)c1)C(c1cccn1)C1CC1</chem>	MCULE MCULE-2202548379
	<chem>Cc1ccnc(N2CCc3cc(C(=O)O)ccc3C2)n1</chem>	MCULE MCULE-3200882870
	<chem>COc1ccccc1NC(=O)c1cc2c(N(C)C)ncnc2c1</chem>	MCULE MCULE-9282439056

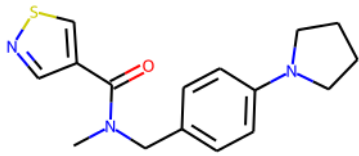
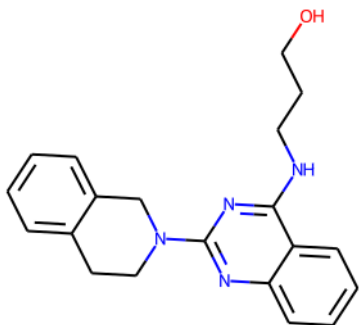
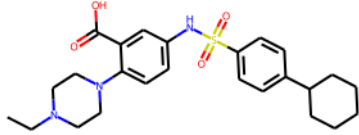
Chemical Structure	SMILES	Vendor
	<chem>CC1C(=O)NCCCN1C(=O)c1ccc2c(N)ncnc2c1</chem>	MCULE MCULE-2190782010
	<chem>O=C(Nc1ccccc1)c1ccc2c(=O)n3c(nc2c1)CCCCC3</chem>	MCULE MCULE-2823588549
	<chem>CC(=O)c1ccc(NC(=O)C2CC(=O)Nc3nc(N4CCc5ccccc5C4)nc(O)c32)cc1</chem>	MCULE MCULE-7270496180

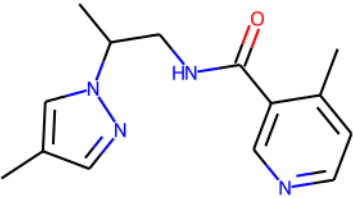
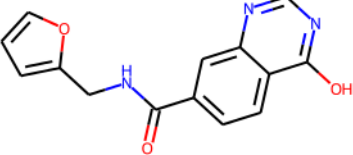
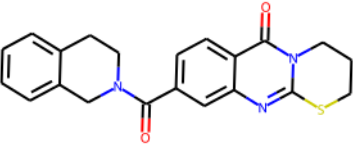
Chemical Structure	SMILES	Vendor
	<chem>CNc1ncnc2cc(C(=O)NC3(c4ccc5c(c4)OCO5)CC3)ccc12</chem>	MCULE MCULE-3903455189
	<chem>CN1CCO[C@@H]2CN(C(=O)c3ccc4[nH]c(=O)[nH]c4c3)C[C@H]21</chem>	MCULE MCULE-9191966569
	<chem>Cc1ccc(NC(=O)N2CCc3nc(N4CCOCC4)nc(N(C)C)c3C2)cc1</chem>	MCULE MCULE-1328390974

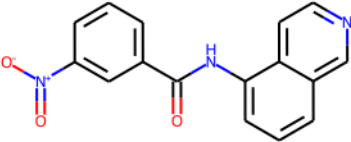
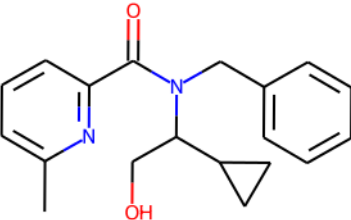
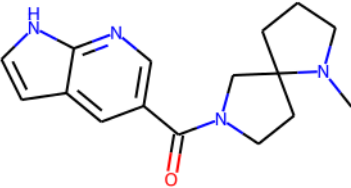
Chemical Structure	SMILES	Vendor
	<chem>CNC(=O)c1ccc(CN2C[C@H]3CCN(C)[C@@H]3C2)cc1</chem>	MCULE MCULE-1518699206
	<chem>O=C1Cc2cc(NC(=O)NCCN3CCCC(c4ccccc4)C3)ccc2N1</chem>	MCULE MCULE-9526301225
	<chem>COc1ccc2c(c1)CN(c1cc(-n3nc(C)cc3N)ncn1)CC2</chem>	MCULE MCULE-3662392776

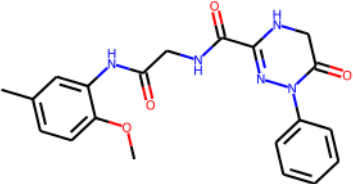
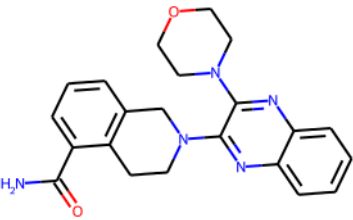
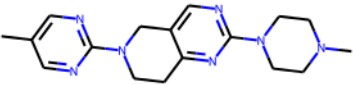
Chemical Structure	SMILES	Vendor
	<chem>CN1CCN(C(=O)c2ccc(NC(=O)CC#N)cc2)CC1</chem>	MCULE MCULE-4607948790
	<chem>COc1cc2c(cc1OC)CN(c1cc(N3CCOCC3)nc(N)n1)CC2</chem>	MCULE MCULE-3863638608
	<chem>Cc1n[nH]c2ccc(C(=O)N(C)CCN(C)C)cc12</chem>	MCULE MCULE-7383634179

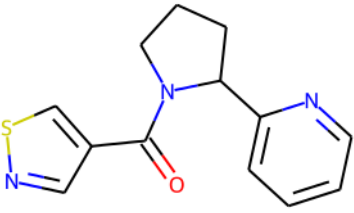
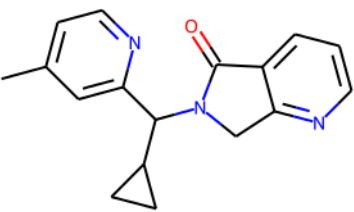
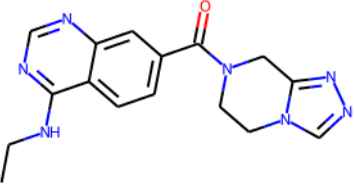
Chemical Structure	SMILES	Vendor
	<chem>N#CCCN(Cc1ccnc1)C(=O)c1ccc2c(=O)[nH]cnc2c1</chem>	MCULE MCULE-5020728369
	<chem>CN1CCCC(O)(CNC2(c3ccccc3)CC2)C1=O</chem>	MCULE MCULE-4499993097
	<chem>CCn1cnnc1CNS(=O)(=O)c1ccc(C(=O)C)cc1</chem>	MCULE MCULE-2097776109

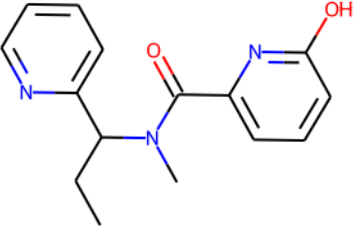
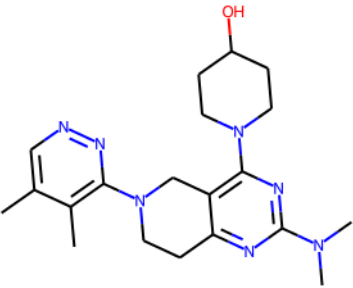
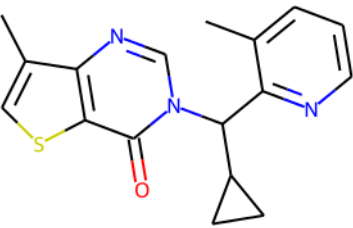
Chemical Structure	SMILES	Vendor
	<chem>CN(Cc1ccc(N2CCCC2)cc1)C(=O)c1cnsc1</chem>	MCULE MCULE-4091995187
	<chem>OCCCNc1nc(N2CCc3cccc(c3C2)nc2ccccc12</chem>	MCULE MCULE-7280647384
	<chem>CCN1CCN(c2ccc(NS(=O)(=O)c3ccc(C4CCCCC4)c(c3)cc2C(=O)O)CC1</chem>	MCULE MCULE-6634136893

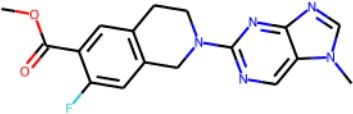
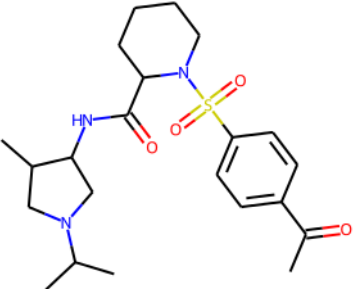
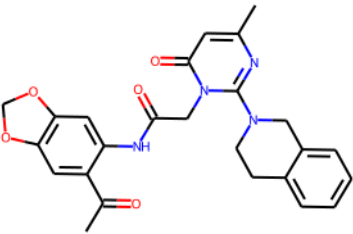
Chemical Structure	SMILES	Vendor
	<chem>Cc1cnn(C(C)C)C(=O)c2cnccc2C)c1</chem>	MCULE MCULE-6665913877
	<chem>O=C(NCc1ccco1)c1ccc2c(O)ncnc2c1</chem>	MCULE MCULE-1413791049
	<chem>O=C(c1ccc2c(=O)n3c(nc2c1)SCCC3)N1CCc2ccccc2C1</chem>	MCULE MCULE-5882759985

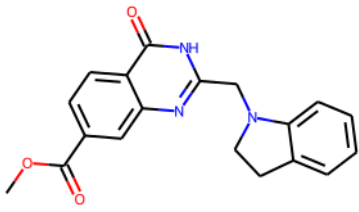
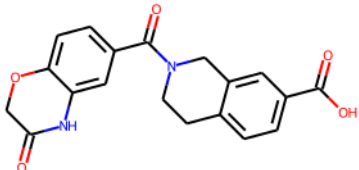
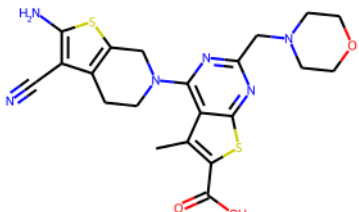
Chemical Structure	SMILES	Vendor
	<chem>O=C(Nc1cccc2cnccc12)c1ccc([N+](=O)[O-])c1</chem>	MCULE MCULE-8572853695
	<chem>Cc1cccc(C(=O)N(Cc2ccccc2)C(CO)C2CC2)n1</chem>	MCULE MCULE-5143170587
	<chem>CN1CCCC12CCN(C(=O)c1cnc3[nH]ccc3c1)C2</chem>	MCULE MCULE-3075427450

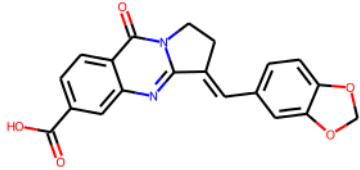
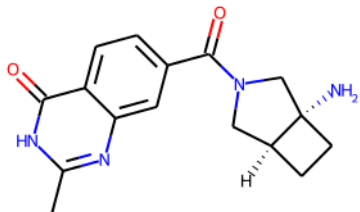
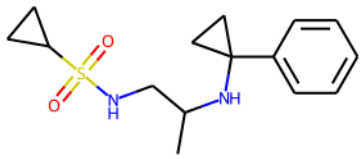
Chemical Structure	SMILES	Vendor
	<chem>COc1ccc(C)cc1NC(=O)CNC(=O)C1=NN(c2ccccc2)C(=O)CN1</chem>	MCULE MCULE-1537903832
	<chem>NC(=O)c1cccc2c1CCN(c3nc3cccc3nc1N1CCOCC1)C2</chem>	MCULE MCULE-5108940804
	<chem>Cc1cnc(N2CCc3nc(N4CCN(C)CC4)nc3)nc1</chem>	MCULE MCULE-8757923239

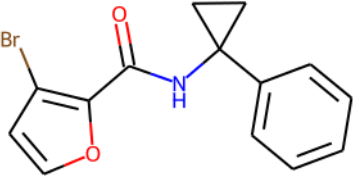
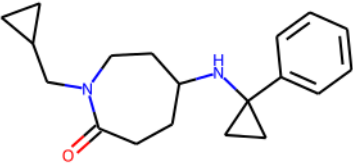
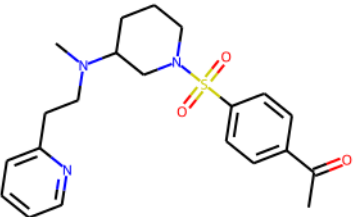
Chemical Structure	SMILES	Vendor
	<chem>O=C(c1cnsc1)N1CCCC1c1cccn1</chem>	MCULE MCULE-9621761161
	<chem>Cc1ccnc(C(C2CC2)N2Cc3ncccc3C2=O)c1</chem>	MCULE MCULE-6948707934
	<chem>CCNc1ncnc2cc(C(=O)N3CCn4cnnc4C3)ccc12</chem>	MCULE MCULE-9827291479

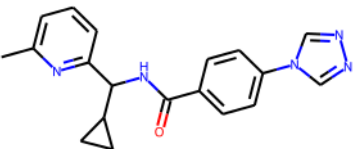
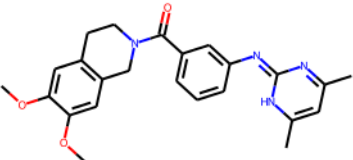
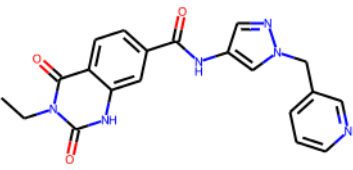
Chemical Structure	SMILES	Vendor
	<chem>CCC(c1ccccn1)N(C)C(=O)c1cccc(O)n1</chem>	MCULE MCULE-9848411541
	<chem>Cc1ennnc(N2CCc3nc(N(C)C)nc(N4CCC(O)CC4)c3C2)c1C</chem>	MCULE MCULE-7960601862
	<chem>Cc1cccnc1C(C1CC1)n1cnc2c(C)csc2c1=O</chem>	MCULE MCULE-6469106048

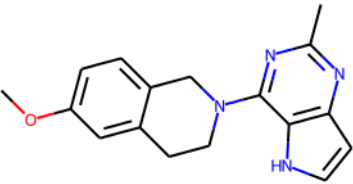
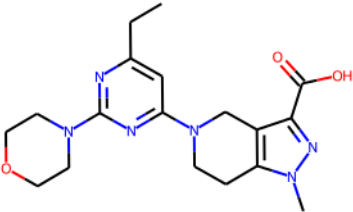
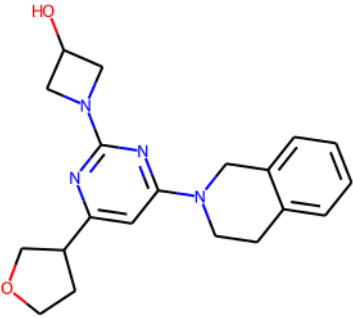
Chemical Structure	SMILES	Vendor
	<chem>COC(=O)c1cc2c(cc1F)C N(c1ncc3c(ncn3C)n1)CC2</chem>	MCULE MCULE-6255084850
	<chem>CC(=O)c1ccc(S(=O)(=O))N2CCCCC2C(=O)NC2CN(C(C)C)CC2C)cc1</chem>	MCULE MCULE-8367745465
	<chem>CC(=O)c1cc2c(cc1NC(=O) Cn1c(N3CCc4ccccc4C 3)nc(C)cc1=O)OCO2</chem>	MCULE MCULE-4794921241

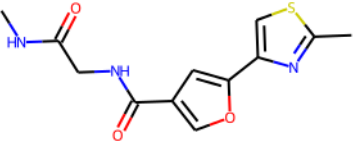
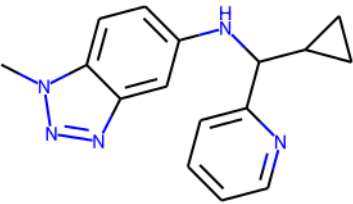
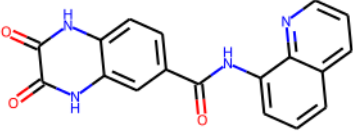
Chemical Structure	SMILES	Vendor
	<chem>COC(=O)c1ccc2c(=O)[nH]c(CN3CCC4CCCCC43)nc2c1</chem>	MCULE MCULE-5732244303
	<chem>O=C1COc2ccc(C(=O)N3CCc4ccc(C(=O)O)cc4C3)cc2N1</chem>	MCULE MCULE-1447433441
	<chem>Cc1c(C(=O)O)sc2nc(CN3CCOCC3)nc(N3CCc4c(s c(N)c4C#N)C3)c12</chem>	MCULE MCULE-1698349537

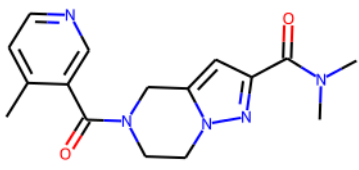
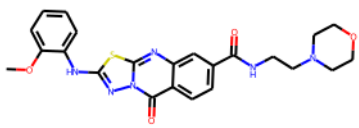
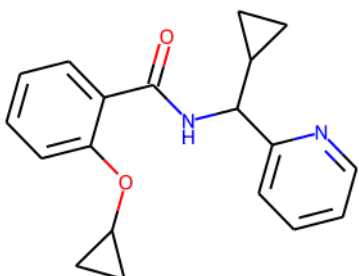
Chemical Structure	SMILES	Vendor
	<chem>O=C(O)c1ccc2c(=O)n3c(nc2c1)C(=Cc1ccc2c(c1)OCO2)CC3</chem>	MCULE MCULE-4854530453
	<chem>Cc1nc2cc(C(=O)N3C[C@H]4CC[C@H]4N3)ccc2c(=O)[nH]1</chem>	MCULE MCULE-5777003027
	<chem>CC(CNS(=O)(=O)C1CC1)NC1(c2ccccc2)CC1</chem>	MCULE MCULE-9640885932

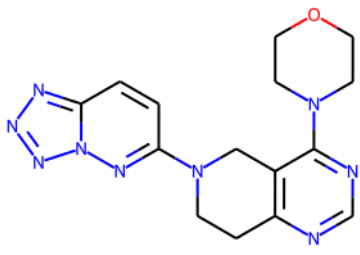
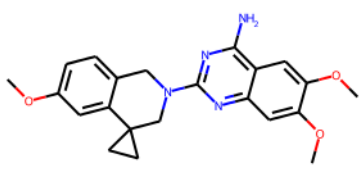
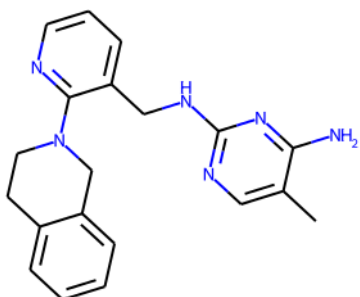
Chemical Structure	SMILES	Vendor
	<chem>O=C(NC1(c2ccccc2)CC1)c1occc1Br</chem>	MCULE MCULE-6437373907
	<chem>O=C1CCC(NC2(c3ccccc3)CC2)CCN1CC1CC1</chem>	MCULE MCULE-1951341405
	<chem>CC(=O)c1ccc(S(=O)(=O)N2CCCC(N2C)CCc3ccccc3)cc1</chem>	MCULE MCULE-7109176142

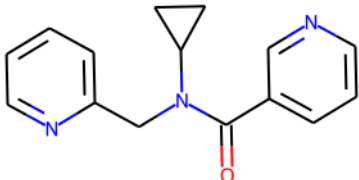
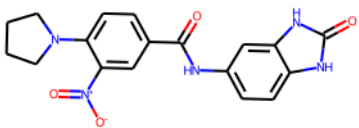
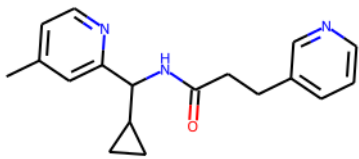
Chemical Structure	SMILES	Vendor
	<chem>Cc1cccc(C(NC(=O)c2ccc(-n3cnnc3)cc2)C2CC2)n1</chem>	MCULE MCULE-1537625185
	<chem>COc1cc2c(cc1OC)CN(C(=O)c1cccc(/N=c3/nc(C)cc(C)[nH]3)c1)CC2</chem>	MCULE MCULE-4610275567
	<chem>CCn1c(=O)[nH]c2cc(C(=O)Nc3cnn(Cc4ccnc4)c3)ccc2c1=O</chem>	MCULE MCULE-6252756189

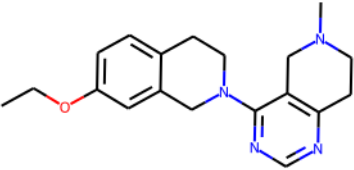
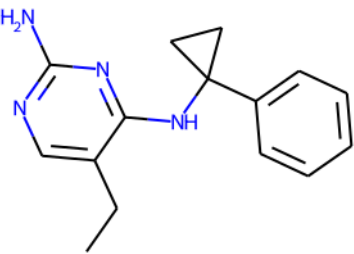
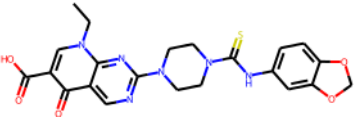
Chemical Structure	SMILES	Vendor
	<chem>COc1ccc2c(c1)CCN(c1ncc(C)[nH]c13)C2</chem>	MCULE MCULE-5708154147
	<chem>CCc1cc(N2CCc3c(c(C(=O)O)O)nn3C)C2)nc(N2CCOCC2)n1</chem>	MCULE MCULE-8641707909
	<chem>OC1CN(c2nc(C3CCOC3)c(N3CCc4ccccc4C3)n2)C1</chem>	MCULE MCULE-4578881101

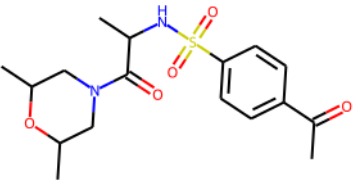
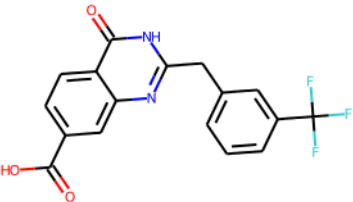
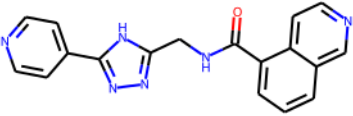
Chemical Structure	SMILES	Vendor
	<chem>CNC(=O)CNC(=O)c1coc(-c2csc(C)n2)c1</chem>	MCULE MCULE-6195753710
	<chem>Cn1nnc2cc(NC(c3cccn3)C3CC3)ccc21</chem>	MCULE MCULE-9585794494
	<chem>O=C(Nc1cccc2cccnc12)c1ccc2[nH]c(=O)c(=O)[nH]c2c1</chem>	MCULE MCULE-8741975998

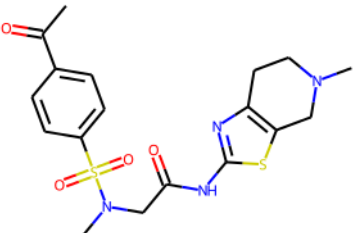
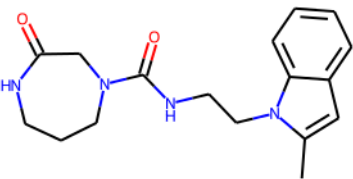
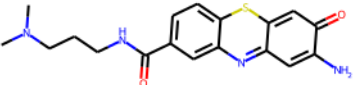
Chemical Structure	SMILES	Vendor
	<chem>Cc1ccncc1C(=O)N1CCn2nc(C(=O)N(C)C)cc2C1</chem>	MCULE MCULE-9228155315
	<chem>COc1cccc1Nc1nn2c(=O)c3ccc(C(=O)NCCN4CCOCC4)cc3nc2s1</chem>	MCULE MCULE-8048668844
	<chem>O=C(NC(c1cccn1)C1CC1)c1cccc1OC1CC1</chem>	MCULE MCULE-7673925253

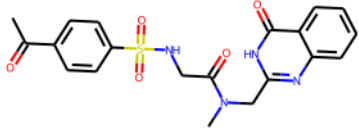
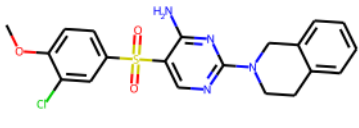
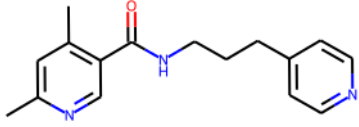
Chemical Structure	SMILES	Vendor
	<chem>c1nc2c(c(N3CCOCC3)n1)CN(c1ccc3nnnn3n1)CC2</chem>	MCULE MCULE-9981542820
	<chem>COc1ccc2c(c1)C1(CC1)CN(c1nc(N)c3cc(OC)c(OC)cc3n1)C2</chem>	MCULE MCULE-2631660057
	<chem>Cc1cnc(NCc2ccnc2N2Cc3ccccc3C2)nc1N</chem>	MCULE MCULE-8915711492

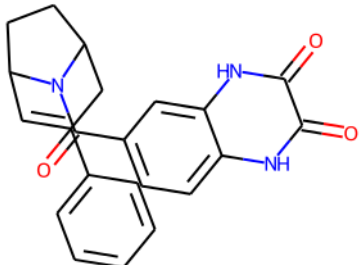
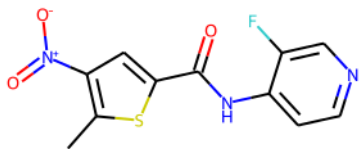
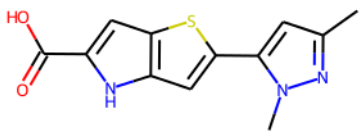
Chemical Structure	SMILES	Vendor
	<chem>O=C(c1ccccc1)N(Cc1ccccc1)C1CC1</chem>	MCULE MCULE-7417207806
	<chem>O=C(Nc1ccc2[nH]c(=O)[nH]c2c1)c1ccc(N2CCC(C2)c([N+](=O)[O-])c1</chem>	MCULE MCULE-6526071201
	<chem>Cc1ccnc(C(NC(=O)CCc2ccccc2)C2CC2)c1</chem>	MCULE MCULE-8665914095

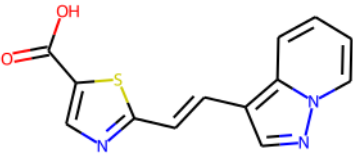
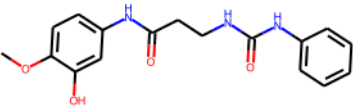
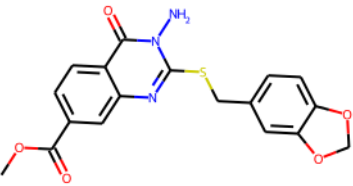
Chemical Structure	SMILES	Vendor
	<chem>CCOc1ccc2c(c1)CN(c1nnc3c1CN(C)CC3)CC2</chem>	MCULE MCULE-3604538379
	<chem>CCc1nc(N)nc1NC1(c2ccccc2)CC1</chem>	MCULE MCULE-8850156723
	<chem>CCn1cc(C(=O)O)c(=O)c2nc(N3CCN(C(=S)Nc4c5cc5c(c4)OCO5)CC3)nc21</chem>	MCULE MCULE-8897625189

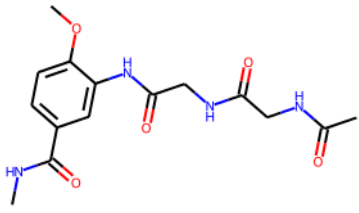
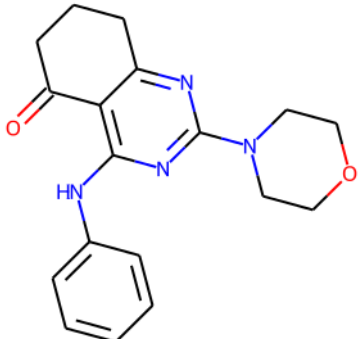
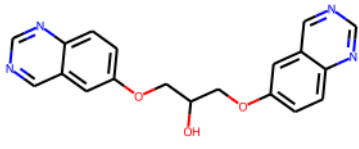
Chemical Structure	SMILES	Vendor
	<chem>CC(=O)c1ccc(S(=O)(=O)NC(C)C(=O)N2CC(C)OC(C)C2)cc1</chem>	MCULE MCULE-8995181174
	<chem>O=C(O)c1ccc2c(=O)[nH]c(nc21)Cc3ccc(C(F)(F)F)cc3</chem>	MCULE MCULE-2426182224
	<chem>O=C(NCc1nnc(-c2ccncc2)[nH]1)c3cccc2ncccc12</chem>	MCULE MCULE-3225846981

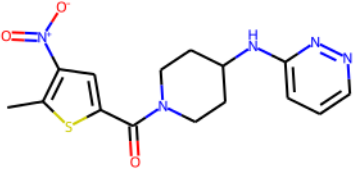
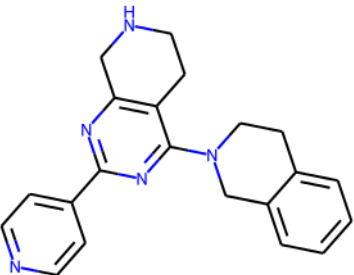
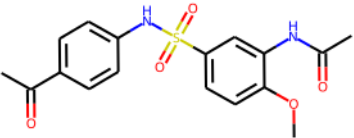
Chemical Structure	SMILES	Vendor
	<chem>CC(=O)c1ccc(S(=O)(=O)N(C)CC(=O)Nc2nc3c(s2)CN(C)CC3)cc1</chem>	MCULE MCULE-8609330840
	<chem>Cc1cc2ccccc2n1CCNC(=O)N1CCCCNC(=O)C1</chem>	MCULE MCULE-6590099945
	<chem>CN(C)CCCNC(=O)c1ccc2sc3cc(=O)c(N)cc-3nc2c1</chem>	MCULE MCULE-5523892558

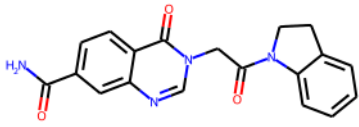
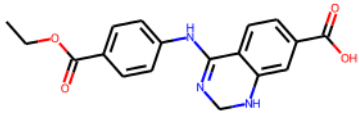
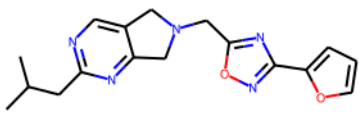
Chemical Structure	SMILES	Vendor
	<chem>CC(=O)c1ccc(S(=O)(=O)NCC(=O)N(C)Cc2nc3ccccc3c(=O)[nH]2)cc1</chem>	MCULE MCULE-4738077028
	<chem>COc1ccc(S(=O)(=O)c2nc(N)nc3c2Cc4ccccc4C3)nc2N)cc1Cl</chem>	MCULE MCULE-1323421898
	<chem>Cc1cc(C)c(C(=O)NCCCC2CCNCC2)cn1</chem>	MCULE MCULE-6290924760

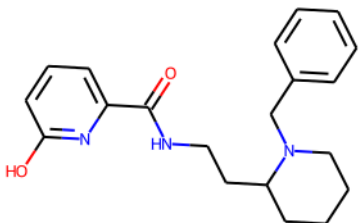
Chemical Structure	SMILES	Vendor
	<chem>O=C(c1ccc2[nH]c(=O)c(=O)[nH]c2c1)N1C2C=C(c3ccccc3)CC1CC2</chem>	MCULE MCULE-7419976972
	<chem>Cc1sc(C(=O)Nc2ccncc2F)cc1[N+](=O)[O-]</chem>	MCULE MCULE-9819111041
	<chem>Cc1cc(-c2cc3[nH]c(C(=O)O)cc3s2)n(C)n1</chem>	MCULE MCULE-7950700891

Chemical Structure	SMILES	Vendor
	<chem>O=C(O)c1cnc(C=Cc2cnn3ccccc23)s1</chem>	MCULE MCULE-3672016639
	<chem>COc1ccc(NC(=O)CCNC(=O)Nc2ccccc2)cc1O</chem>	MCULE MCULE-4790126168
	<chem>COC(=O)c1ccc2c(=O)n(N)c(SCc3ccc4c(c3)OCO4)nc2c1</chem>	MCULE MCULE-3403128906

Chemical Structure	SMILES	Vendor
	<chem>CNC(=O)c1ccc(OC)c(NC(=O)CNC(=O)CNC(C)=O)c1</chem>	MCULE MCULE-9754715793
	<chem>O=C1CCCC2Nc(N3CCOCC3)nc(Nc3ccccc3)c21</chem>	MCULE MCULE-5643537369
	<chem>OC(COc1ccc2ncncc2c1)COc1ccc2ncncc2c1</chem>	MCULE MCULE-6845932737

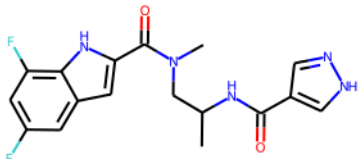
Chemical Structure	SMILES	Vendor
	<chem>Cc1sc(C(=O)N2CCC(Nc3ccnn3)CC2)cc1[N+](=O)[O-]</chem>	MCULE MCULE-1449396541
	<chem>c1ccc2c(c1)CCN(c1nc(-c3ccncc3)nc3c1CCNC3)C2</chem>	MCULE MCULE-2164297195
	<chem>COc1ccc(S(=O)(=O)Nc2ccc(C(=O)N)cc2)cc1NC(C)=O</chem>	MCULE MCULE-3149295740

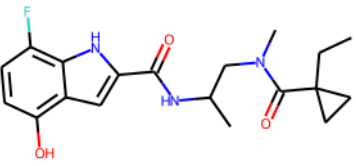
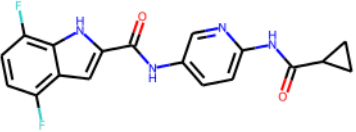
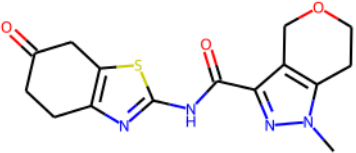
Chemical Structure	SMILES	Vendor
	<chem>NC(=O)c1ccc2c(=O)n(C(=O)N3CCc4cccc43)cnc2c1</chem>	MCULE MCULE-6703109920
	<chem>CCOC(=O)c1ccc(NC2=NC3C=CC(=O)O)cc32</chem>	MCULE MCULE-4466264677
	<chem>CC(C)Cc1ncc2c(n1)CN(Cc1nc(-c3ccco3)no1)C2</chem>	MCULE MCULE-8855197724

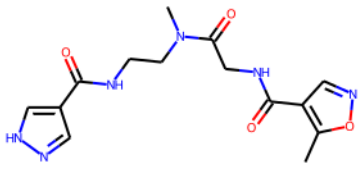
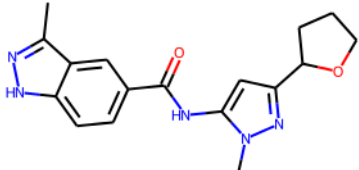
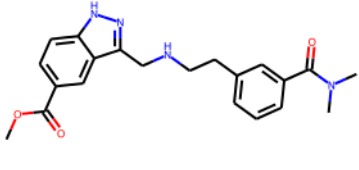
Chemical Structure	SMILES	Vendor
	<chem>O=C(NCCCC1CCCCN1Cc1cccc(O)n1</chem>	MCULE MCULE-4698385990

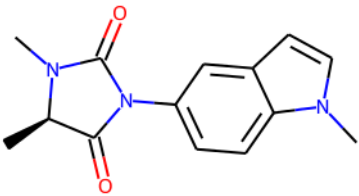
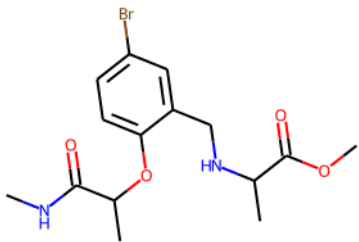
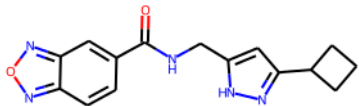
5 TRIM9

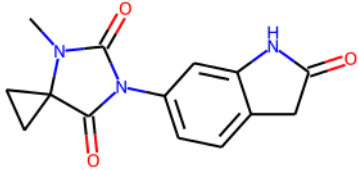
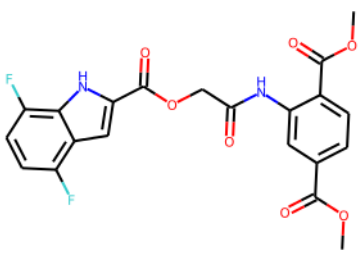
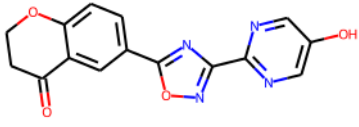
UniProtKB entry Q9C026

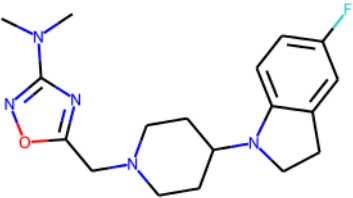
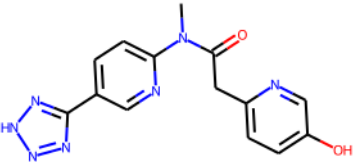
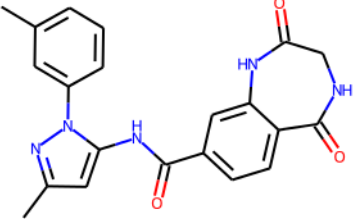
Chemical Structure	SMILES	Vendor
	<chem>CC(CN(C)C(=O)c1cc2cc(F)cc(F)c2[nH]1)NC(=O)c1cn[nH]c1</chem>	ENAMINE PV-004024184545

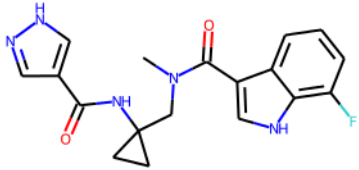
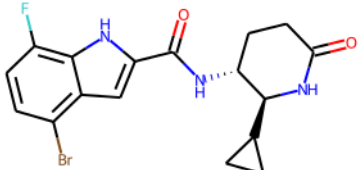
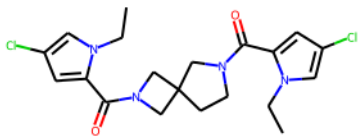
Chemical Structure	SMILES	Vendor
	<chem>CCC1(C(=O)N(C)CC(C)N</chem> <chem>C(=O)c2cc3c(O)ccc(F)c3[nH]2)CC1</chem>	ENAMINE PV-003983238946
	<chem>O=C(Nc1ccc(NC(=O)C2C</chem> <chem>C2)nc1)c1cc2c(F)ccc(F)c2[nH]1</chem>	ENAMINE Z1222833368
	<chem>Cn1nc(C(=O)Nc2nc3c(s</chem> <chem>2)CC(=O)CC3)c2c1CCOC2</chem>	ENAMINE Z4624364873

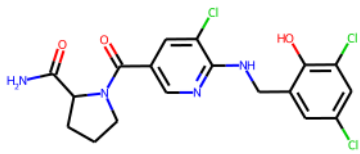
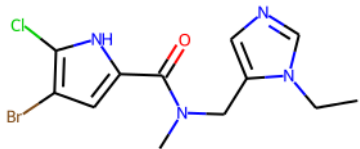
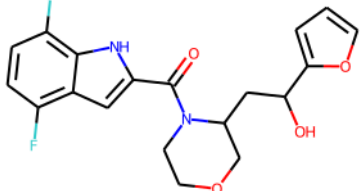
Chemical Structure	SMILES	Vendor
	<chem>Cc1oncc1C(=O)NCC(=O)N(C)CCNC(=O)c1cn[nH]c1</chem>	ENAMINE PV-003265830747
	<chem>Cc1n[nH]c2ccc(C(=O)Nc3cc(C4CCCO4)nn3C)cc12</chem>	ENAMINE Z2637744828
	<chem>COC(=O)c1ccc2[nH]nc(CNCCc3cccc(C(=O)N(C)C)c3)c2c1</chem>	ENAMINE Z4195193559

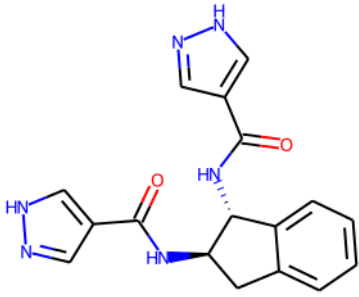
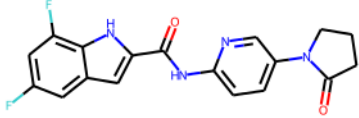
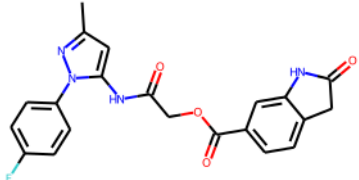
Chemical Structure	SMILES	Vendor
	<chem>C[C@@H]1C(=O)N(c2ccc3c(ccn3C)c2)C(=O)N1C</chem>	ENAMINE Z3499889660
	<chem>CNC(=O)C(C)Oc1ccc(Br)cc1CNC(C)C(=O)OC</chem>	ENAMINE Z2256805937
	<chem>O=C(NCc1cc(C2CCC2)n[nH]1)c1ccc2nonc2c1</chem>	ENAMINE Z3614384658

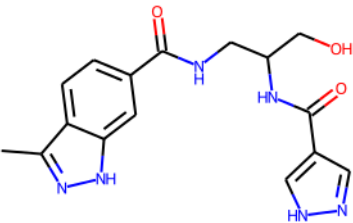
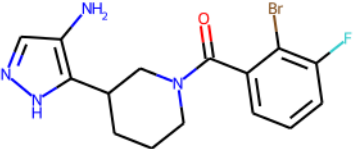
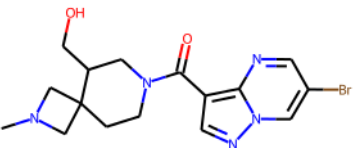
Chemical Structure	SMILES	Vendor
	<chem>CN1C(=O)N(c2ccc3c(c2)NC(=O)C3)C(=O)C12CC2</chem>	ENAMINE Z3349821537
	<chem>COC(=O)c1ccc(C(=O)OC)c(NC(=O)COC(=O)c2cc3c(F)ccc(F)c3[nH]2)c1</chem>	ENAMINE Z1223806978
	<chem>O=C1CCOc2ccc(-c3nc(-c4ncc(O)cn4)no3)cc21</chem>	ENAMINE PV-003204597127

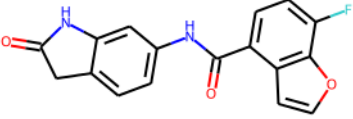
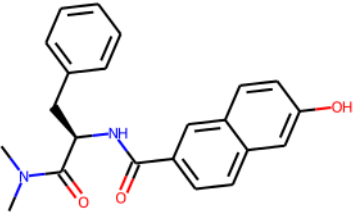
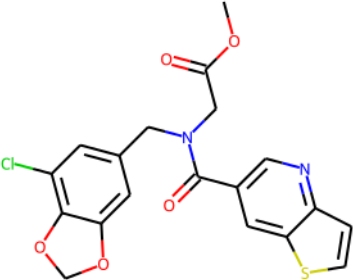
Chemical Structure	SMILES	Vendor
	<chem>CN(C)c1noc(CN2CCC(N3CCc4cc(F)ccc43)CC2)n1</chem>	ENAMINE Z2015738616
	<chem>CN(C(=O)Cc1ccc(O)cn1)c1ccc(-c2nn[nH]n2)cn1</chem>	ENAMINE PV-003005145661
	<chem>Cc1ccc(-n2nc(C)cc2NC(=O)c2ccc3c(c2)NC(=O)CNC3=O)c1</chem>	ENAMINE Z2220289001

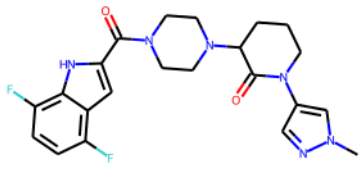
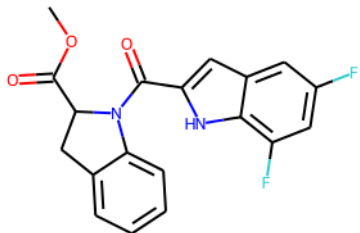
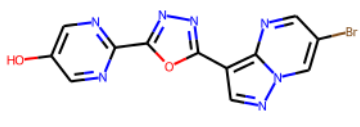
Chemical Structure	SMILES	Vendor
	<chem>CN(CC1(NC(=O)c2cn[nH]c2)CC1)C(=O)c1c[nH]c2c(F)cccc12</chem>	ENAMINE PV-003823311789
	<chem>O=C1CC[C@H](NC(=O)c2cc3c(Br)ccc(F)c3[nH]2)[C@H](C2CC2)N1</chem>	ENAMINE Z3671630650
	<chem>CCn1cc(Cl)cc1C(=O)N1CCC2(C1)CN(C(=O)c1cc(Cl)cn1CC)C2</chem>	ENAMINE Z4879516018

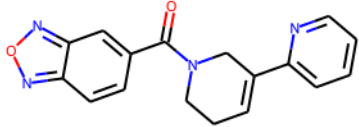
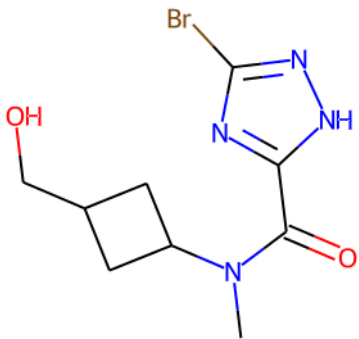
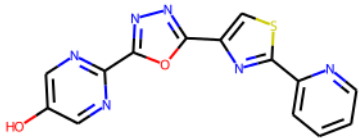
Chemical Structure	SMILES	Vendor
	<chem>NC(=O)C1CCCN1C(=O)c1cnc(NCc2cc(Cl)cc(Cl)c2O)c(Cl)c1</chem>	ENAMINE Z2143433731
	<chem>CCn1cncc1CN(C)C(=O)c1cc(Br)c(Cl)[nH]1</chem>	ENAMINE Z3612430213
	<chem>O=C(c1cc2c(F)ccc(F)c2[nH]1)N1CCOCC1CC(O)c1ccco1</chem>	ENAMINE Z1433163200

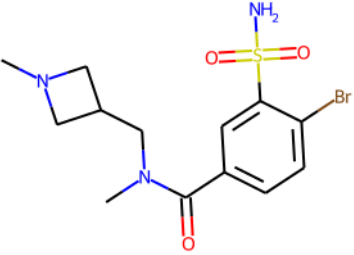
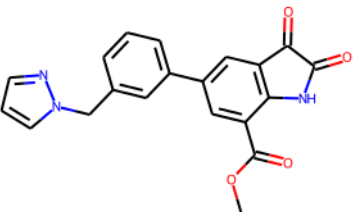
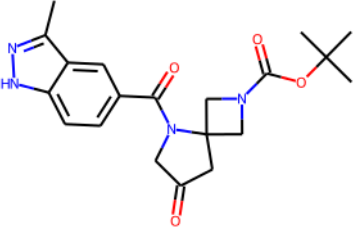
Chemical Structure	SMILES	Vendor
	<chem>O=C(N[C@@H]1Cc2ccccc2[C@H]1NC(=O)c1cn[nH]c1)c1cn[nH]c1</chem>	ENAMINE PV-000233323740
	<chem>O=C(Nc1ccc(N2CCCC2=O)cn1)c1cc2cc(F)cc(F)c2[nH]1</chem>	ENAMINE PV-003005786715
	<chem>Cc1cc(NC(=O)COC(=O)c2ccc3c(c2)NC(=O)C3)n(-c2ccc(F)cc2)n1</chem>	ENAMINE Z1798284827

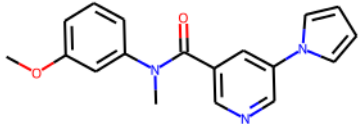
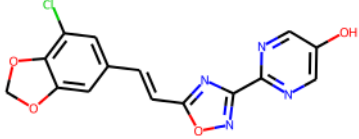
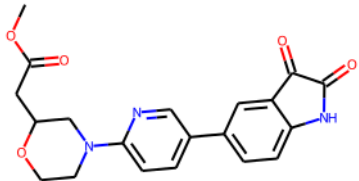
Chemical Structure	SMILES	Vendor
	<chem>Cc1n[nH]c2cc(C(=O)NC(C(O)C)NC(=O)c3cn[nH]c3)ccc12</chem>	ENAMINE PV-003862705203
	<chem>Nc1cn[nH]c1C1CCCN(C(=O)c2cccc(F)c2Br)C1</chem>	ENAMINE Z4176525973
	<chem>CN1CC2(CCN(C(=O)c3cn[n4cc(Br)cnc34)CC2CO)C1</chem>	ENAMINE Z3898850031

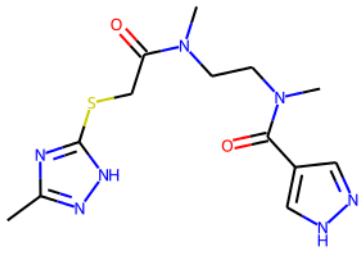
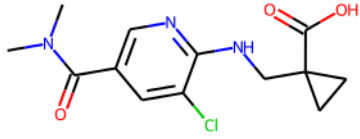
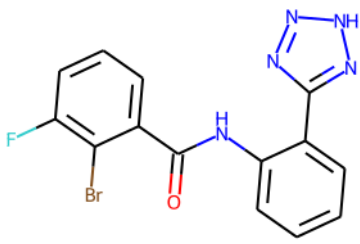
Chemical Structure	SMILES	Vendor
	<chem>O=C1Cc2ccc(NC(=O)c3ccc(F)c4occc34)cc2N1</chem>	ENAMINE PV-002366164370
	<chem>CN(C)C(=O)[C@@H](Cc1ccc(O)cc1)NC(=O)c1ccc2cc(O)ccc2c1</chem>	ENAMINE PV-003962606232
	<chem>COC(=O)CN(Cc1cc(Cl)cc2c1OCO2)C(=O)c1cnc2ccsc2c1</chem>	ENAMINE Z1368115223

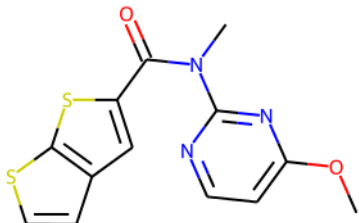
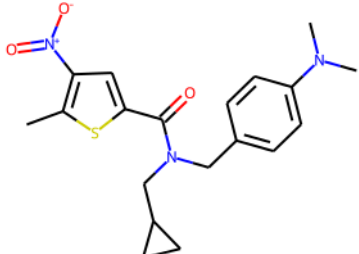
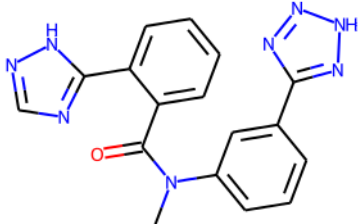
Chemical Structure	SMILES	Vendor
	<chem>Cn1cc(N2CCCC(N3CCN(C(=O)c4cc5c(F)ccc(F)c5[nH]4)CC3)C2=O)cn1</chem>	ENAMINE Z1625809501
	<chem>COC(=O)C1Cc2ccccc2N1C(=O)c1cc2cc(F)cc(F)c2[nH]1</chem>	ENAMINE PV-002768173772
	<chem>Oc1cnc(-c2nnc(-c3cnn4cc(Br)cnc34)o2)nc1</chem>	ENAMINE PV-003964305157

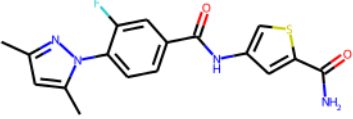
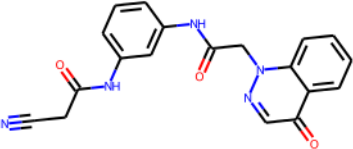
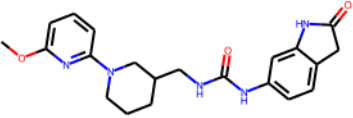
Chemical Structure	SMILES	Vendor
	<chem>O=C(c1ccc2nonc2c1)N1CCC=C(c2cccn2)C1</chem>	ENAMINE PV-002308989162
	<chem>CN(C(=O)c1nc(Br)n[nH]1)C1CC(CO)C1</chem>	ENAMINE Z4414803540
	<chem>Oc1cnc(-c2nnc(-c3csc(-c4cccn4)n3)o2)nc1</chem>	ENAMINE PV-002947184480

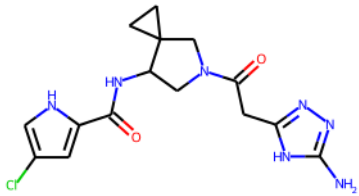
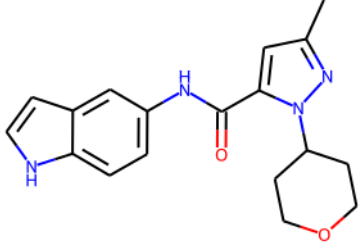
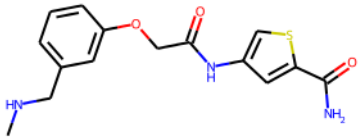
Chemical Structure	SMILES	Vendor
	<chem>CN1CC(CN(C)C(=O)c2cc</chem> <chem>c(Br)c(S(N)(=O)=O)c2)C1</chem>	ENAMINE Z2645159374
	<chem>COC(=O)c1cc(-c2cccc(</chem> <chem>Cn3cccn3)c2)cc2c1NC(=O)C2=O</chem>	ENAMINE Z3484591769
	<chem>Cc1n[nH]c2ccc(C(=O)N</chem> <chem>3CC(=O)CC34CN(C(=O)O</chem> <chem>C(C)(C)C)C4)cc12</chem>	ENAMINE Z3625259642

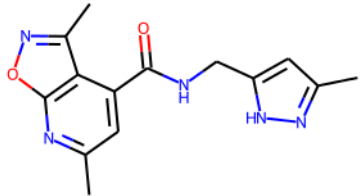
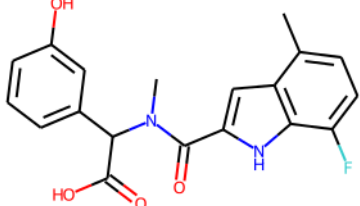
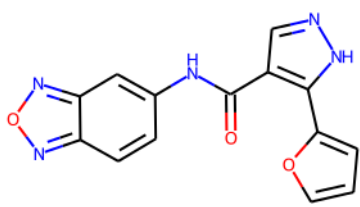
Chemical Structure	SMILES	Vendor
	<chem>COc1cccc(N(C)C(=O)c2cncc(-n3cccc3)c2)c1</chem>	ENAMINE PV-002754542118
	<chem>Oc1cnc(-c2noc(C=Cc3cc(Cl)c4c(c3)OCO4)n2)nc1</chem>	ENAMINE PV-003232543598
	<chem>COC(=O)CC1CN(c2ccc(-c3ccc4c(c3)C(=O)C(=O)N4)cn2)CCO1</chem>	ENAMINE Z3347750986

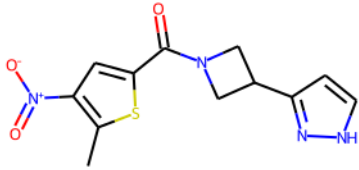
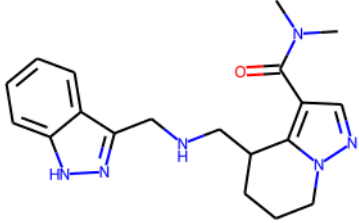
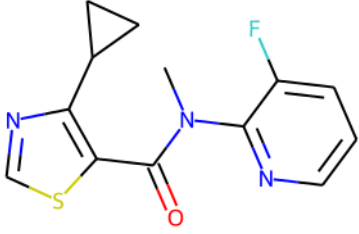
Chemical Structure	SMILES	Vendor
	<chem>Cc1n[nH]c(SCC(=O)N(C)CCN(C)C(=O)c2cn[nH]c2)n1</chem>	ENAMINE PV-002910471125
	<chem>CN(C)C(=O)c1cnc(NCC2(C(=O)O)CC2)c(Cl)c1</chem>	ENAMINE Z3496366045
	<chem>O=C(Nc1ccccc1-c1nn[nH]n1)c1cccc(F)c1Br</chem>	ENAMINE PV-002452967390

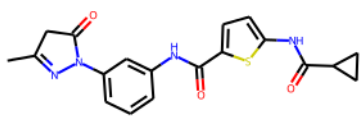
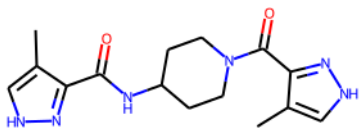
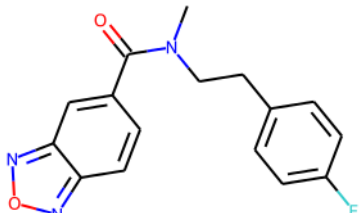
Chemical Structure	SMILES	Vendor
	<chem>COc1ccnc(N(C)C(=O)c2cc3ccsc3s2)n1</chem>	ENAMINE PV-002141104048
	<chem>Cc1sc(C(=O)N(Cc2ccc(N(C)C)cc2)CC2CC2)cc1[N+](=O)[O-]</chem>	ENAMINE Z1129157048
	<chem>CN(C(=O)c1ccccc1-c1n[nH]1)c2cc(-c2nn[nH]n2)c1</chem>	ENAMINE PV-002916202727

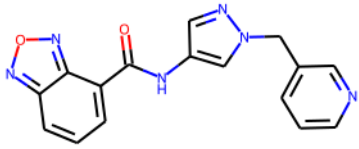
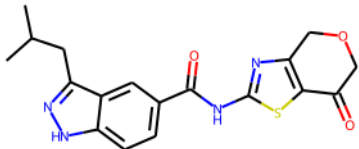
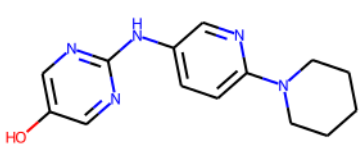
Chemical Structure	SMILES	Vendor
	<chem>Cc1cc(C)n(-c2ccc(C(=O)Nc3csc(C(N)=O)c3)cc2F)n1</chem>	ENAMINE PV-002146588557
	<chem>N#CCCC(=O)Nc1cccc(NC(=O)Cn2ncc(=O)c3ccccc32)c1</chem>	ENAMINE PV-003960961599
	<chem>COc1cccc(N2CCCC(CNC(=O)Nc3ccc4c(c3)NC(=O)C4)C2)n1</chem>	ENAMINE Z4466407245

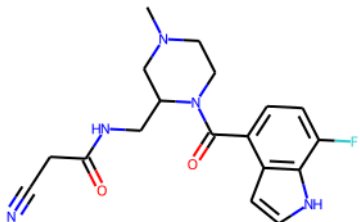
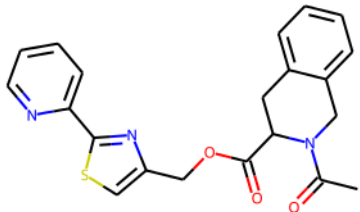
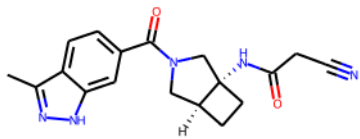
Chemical Structure	SMILES	Vendor
	<chem>Nc1nnc(CC(=O)N2CC(NC(=O)c3cc(Cl)c[nH]3)C3(CC3)C2)[nH]1</chem>	ENAMINE PV-003991813677
	<chem>Cc1cc(C(=O)Nc2ccc3[nH]ccc3c2)n(C2CCOCC2)n1</chem>	ENAMINE Z2698374308
	<chem>CNCc1cccc(OCC(=O)Nc2csc(C(N)=O)c2)c1</chem>	ENAMINE PV-003227617208

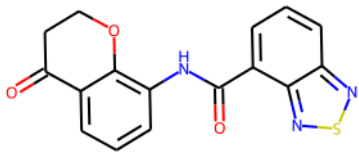
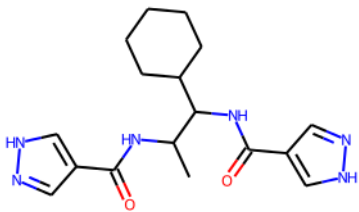
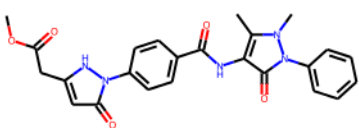
Chemical Structure	SMILES	Vendor
	<chem>Cc1cc(CNC(=O)C2CC(C)NC3ONC(C)C23)[nH]n1</chem>	ENAMINE Z1193211634
	<chem>Cc1ccc(F)c2[nH]c(C(=O)N(C)C(C(=O)O)c3cccc(O)c3)cc12</chem>	ENAMINE PV-003592725635
	<chem>O=C(Nc1ccc2nonc2c1)c1cn[nH]c1-c1ccco1</chem>	ENAMINE PV-002748077612

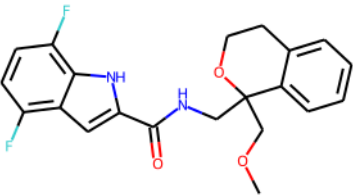
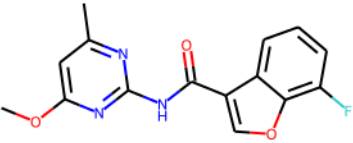
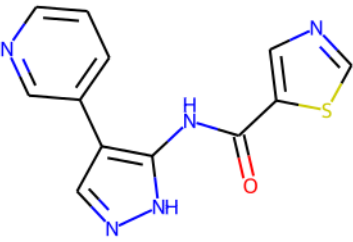
Chemical Structure	SMILES	Vendor
	<chem>Cc1sc(C(=O)N2CC(c3cc[nH]n3)C2)cc1[N+](=O)[O-]</chem>	ENAMINE Z3592157181
	<chem>CN(C)C(=O)c1cnn2c1C(CNCc1n[nH]c3ccccc13)CCC2</chem>	ENAMINE Z2382009664
	<chem>CN(C(=O)c1scnc1C1CC1)c1ncccc1F</chem>	ENAMINE Z1533847571

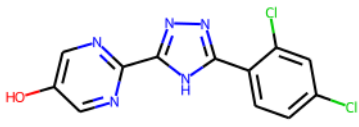
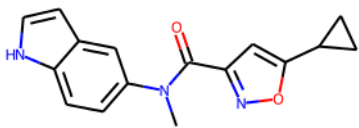
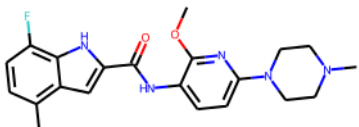
Chemical Structure	SMILES	Vendor
	<chem>CC1=NN(c2cccc(NC(=O)c3ccc(NC(=O)C4CC4)s3)c2)C(=O)C1</chem>	ENAMINE Z3367364149
	<chem>Cc1c[nH]nc1C(=O)NC1CCN(C1)C(=O)c2n[nH]cc2C)CC1</chem>	ENAMINE PV-000417404894
	<chem>CN(CCc1ccc(F)cc1)C(=O)c1ccc2nnc2c1</chem>	ENAMINE PV-002306819738

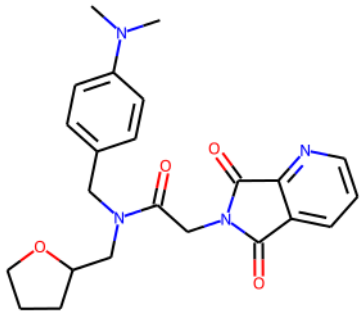
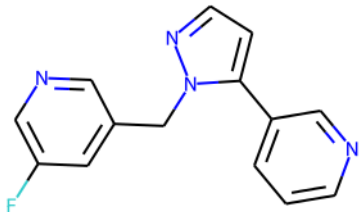
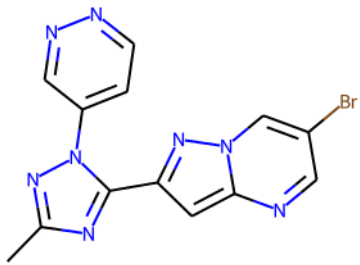
Chemical Structure	SMILES	Vendor
	<chem>O=C(Nc1cnn(Cc2ccccc2)c1)c1cccc2nnc12</chem>	ENAMINE PV-002766200564
	<chem>CC(C)Cc1n[nH]c2ccc(C(=O)Nc3nc4c(s3)C(=O)COC4)cc12</chem>	ENAMINE Z4150643597
	<chem>Oc1cnc(Nc2ccc(N3CCCCC3)nc2)nc1</chem>	ENAMINE Z3075450665

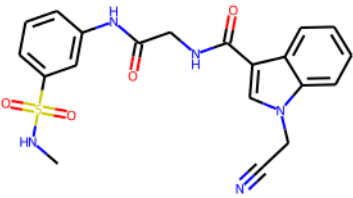
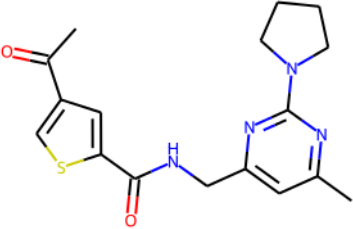
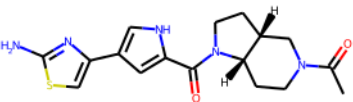
Chemical Structure	SMILES	Vendor
	<chem>CN1CCN(C(=O)c2ccc(F)c3[nH]ccc23)C(CNC(=O)CC#N)C1</chem>	ENAMINE PV-003561548208
	<chem>CC(=O)N1Cc2ccccc2CC1C(=O)OCc1csc(-c2cccn2)n1</chem>	ENAMINE Z1616511031
	<chem>Cc1n[nH]c2cc(C(=O)N3C[C@@H]4CC[C@]4(NC(=O)CC#N)C3)ccc12</chem>	ENAMINE PV-003811351120

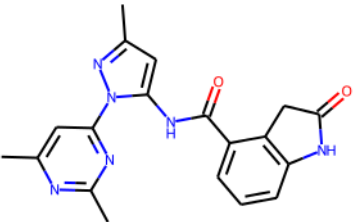
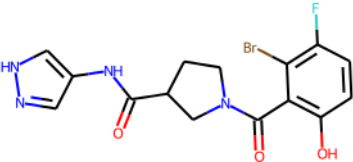
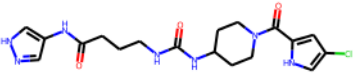
Chemical Structure	SMILES	Vendor
	<chem>O=C1CCOc2c(NC(=O)c3ccccc3nsnc34)cccc21</chem>	ENAMINE PV-001890687241
	<chem>CC(NC(=O)c1cn[nH]c1)C(NC(=O)c1cn[nH]c1)C1CCCCC1</chem>	ENAMINE PV-003614811977
	<chem>COC(=O)Cc1cc(=O)n(-c2ccc(C(=O)Nc3c(C)n(C)n(-c4ccccc4)c3=O)cc2)[nH]1</chem>	ENAMINE Z361941802

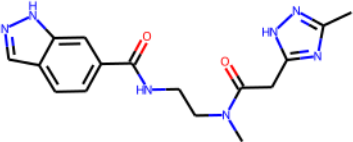
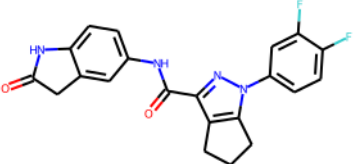
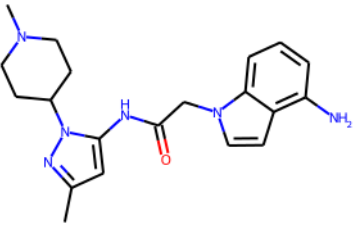
Chemical Structure	SMILES	Vendor
	<chem>COCC1(CNC(=O)c2cc3c(F)ccc(F)c3[nH]2)OCCc2ccccc21</chem>	ENAMINE Z2177997542
	<chem>COc1cc(C)nc(NC(=O)c2cc3cc(F)ccc3o2)n1</chem>	ENAMINE PV-002570767656
	<chem>O=C(Nc1[nH]ncc1-c1ccnc1)c1cnsc1</chem>	ENAMINE PV-002805176325

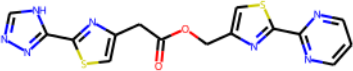
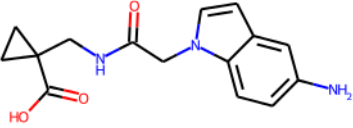
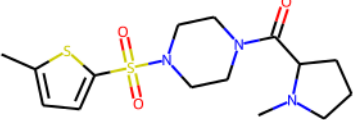
Chemical Structure	SMILES	Vendor
	<chem>Oc1cnc(-c2nnc(-c3ccc(Cl)cc3Cl)[nH]2)nc1</chem>	ENAMINE PV-003880952282
	<chem>CN(C(=O)c1cc(C2CC2)o[nH]1)c1ccc2[nH]ccc2c1</chem>	ENAMINE Z3662296774
	<chem>COc1nc(N2CCN(C)CC2)c[nH]1C(=O)c1cc2c(C)ccc(F)c2[nH]1</chem>	ENAMINE Z2710109118

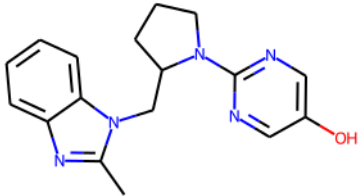
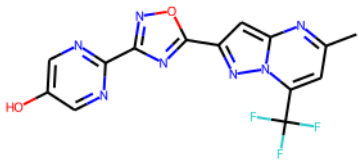
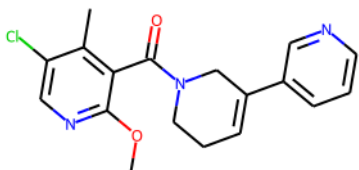
Chemical Structure	SMILES	Vendor
	<chem>CN(C)c1ccc(CN(CC2CCCOC2)C(=O)CN2C(=O)c3ccncc3C2=O)cc1</chem>	ENAMINE Z1167632406
	<chem>Fc1cncc(Cn2nccc2-c2ccncc2)c1</chem>	ENAMINE Z1956749671
	<chem>Cc1nc(-c2cc3ncc(Br)cn3n2)n(-c2ccncc2)n1</chem>	ENAMINE PV-003174797351

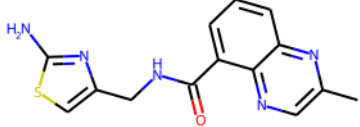
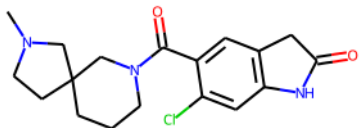
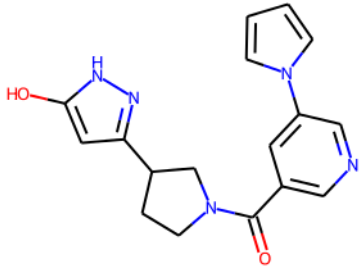
Chemical Structure	SMILES	Vendor
	<chem>CNS(=O)(=O)c1cccc(NC(=O)CNC(=O)c2cn(CC#N)c3ccccc23)c1</chem>	ENAMINE Z1129420882
	<chem>CC(=O)c1csc(C(=O)NCc2cc(C)nc(N3CCCC3)n2)c1</chem>	ENAMINE Z2229934954
	<chem>CC(=O)N1CC[C@H]2[C@H](CCN2C(=O)c2cc(-c3csc(N)n3)c[nH]2)C1</chem>	ENAMINE PV-003152243841

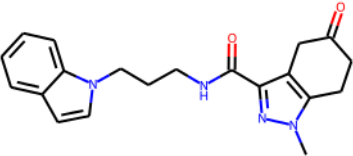
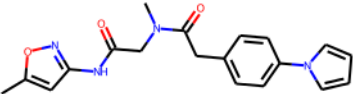
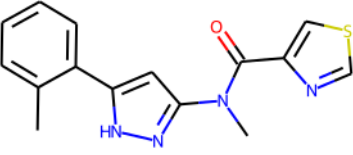
Chemical Structure	SMILES	Vendor
	<chem>Cc1cc(-n2nc(C)cc2NC(=O)c2cccc3c2CC(=O)N3)nc(C)n1</chem>	ENAMINE PV-004006967812
	<chem>O=C(Nc1cn[nH]c1)C1CCN(C(=O)c2c(O)ccc(F)c2Br)C1</chem>	ENAMINE Z4311462069
	<chem>O=C(CCCNC(=O)NC1CCN(C(=O)c2cc(Cl)c[nH]2)CC1)Nc1cn[nH]c1</chem>	ENAMINE Z2115390567

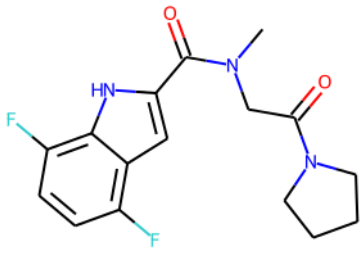
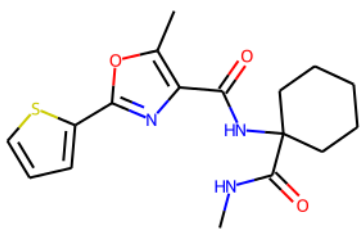
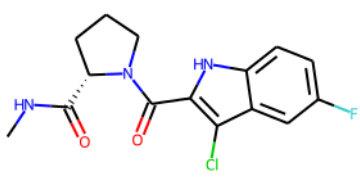
Chemical Structure	SMILES	Vendor
	<chem>Cc1n[nH]c(CC(=O)N(C)CCNC(=O)c2ccc3cn[nH]c3c2)n1</chem>	ENAMINE PV-003040493266
	<chem>O=C1Cc2cc(NC(=O)c3nn(-c4ccc(F)c(F)c4)c3CCC4)ccc2N1</chem>	ENAMINE Z1198958069
	<chem>Cc1cc(NC(=O)Cn2ccc3c(N)cccc32)n(C2CCN(C)CC2)n1</chem>	ENAMINE Z3352027395

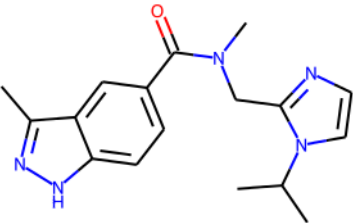
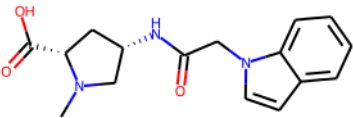
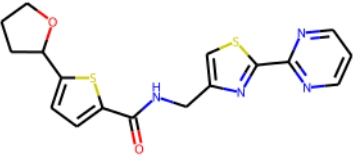
Chemical Structure	SMILES	Vendor
	<chem>O=C(Cc1csc(-c2nnc[nH]2)n1)OCc1csc(-c2ncccn2)n1</chem>	ENAMINE Z1179729198
	<chem>Nc1ccc2c(ccn2CC(=O)NCC2(C(=O)O)CC2)c1</chem>	ENAMINE Z3547977227
	<chem>Cc1ccc(S(=O)(=O)N2CCN(CC2)C(=O)N3CCCC3)s1</chem>	ENAMINE Z968938340

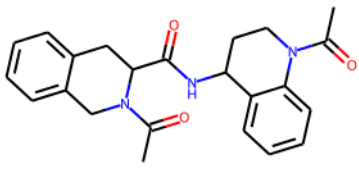
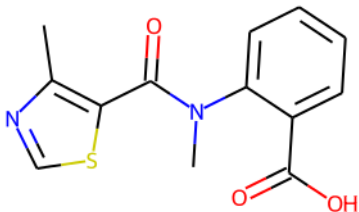
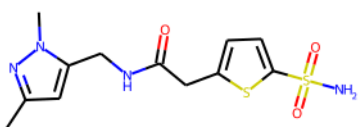
Chemical Structure	SMILES	Vendor
	<chem>Cc1nc2ccccc2n1CC1CCC N1c1ncc(O)cn1</chem>	ENAMINE Z3076509486
	<chem>Cc1cc(C(F)(F)F)n2nc(-c3nc(- c4ncc(O)cn4)no3)cc2n1</chem>	ENAMINE PV-003940188165
	<chem>COc1ncc(Cl)c(C)c1C(=O) N1CCC=C(c2ccncc2)C1</chem>	ENAMINE Z3550127326

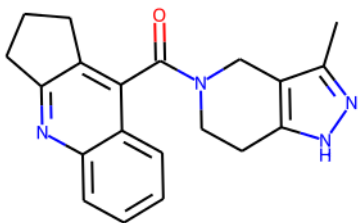
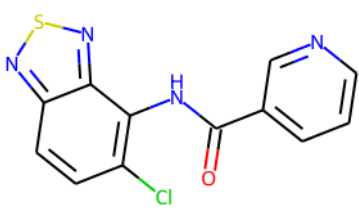
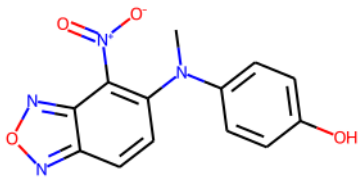
Chemical Structure	SMILES	Vendor
	<chem>Cc1cnc2c(C(=O)NCc3cs</chem> <chem>c(N)n3)cccc2n1</chem>	ENAMINE PV-002917258813
	<chem>CN1CCC2(CCCN(C(=O)c3</chem> <chem>cc4c(cc3Cl)NC(=O)C4)C2)C1</chem>	ENAMINE Z2640813048
	<chem>O=C(c1cncc(-n2cccc2)</chem> <chem>c1)N1CCC(c2cc(O)[nH]n2)C1</chem>	ENAMINE PV-002869963556

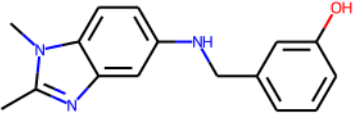
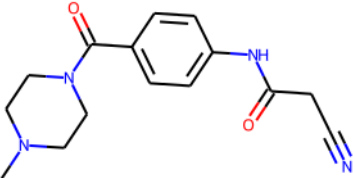
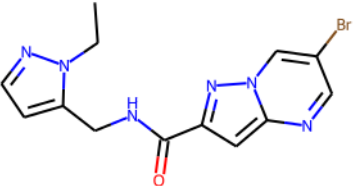
Chemical Structure	SMILES	Vendor
	<chem>Cn1nc(C(=O)NCCCn2ccc3ccccc32)c2c1CCC(=O)C2</chem>	MCULE MCULE-4580753903
	<chem>Cc1cc(NC(=O)CN(C)C(=O)Cc2ccc(-n3cccc3)cc2)no1</chem>	MCULE MCULE-6150069646
	<chem>Cc1ccccc1-c1cc(N(C)C(=O)c2csn2)n[nH]1</chem>	MCULE MCULE-5814949327

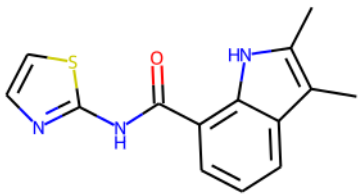
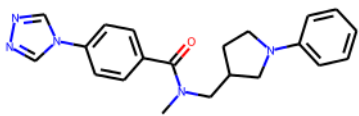
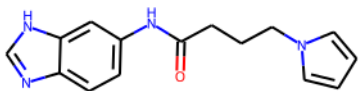
Chemical Structure	SMILES	Vendor
	<chem>CN(CC(=O)N1CCCC1)C(=O)c1cc2c(F)ccc(F)c2[nH]1</chem>	MCULE MCULE-4741865445
	<chem>CNC(=O)C1(NC(=O)c2nc(-c3cccs3)oc2C)CCCC1</chem>	MCULE MCULE-4105920739
	<chem>CNC(=O)[C@@H]1CCCN1C(=O)c1[nH]c2ccc(F)cc2c1Cl</chem>	MCULE MCULE-2435269564

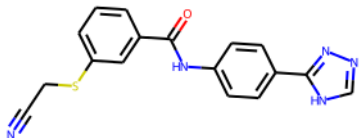
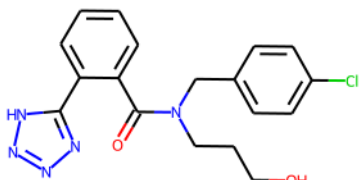

Chemical Structure	SMILES	Vendor
	<chem>Cc1n[nH]c2ccc(C(=O)N(C)Cc3nccn3C(C)C)cc12</chem>	MCULE MCULE-2833056784
	<chem>CN1C[C@@H](NC(=O)Cn2ccc3ccccc32)C[C@H]1C(=O)O</chem>	MCULE MCULE-9263973498
	<chem>O=C(NCc1sc(-c2ncccn2)n1)c1ccc(C2CCCO2)s1</chem>	MCULE MCULE-7572266570

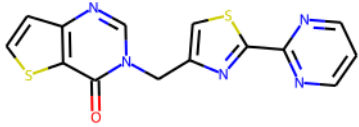
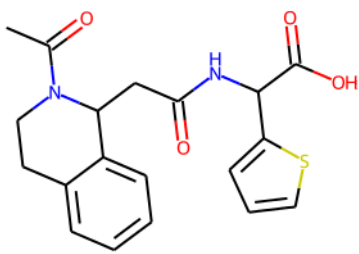
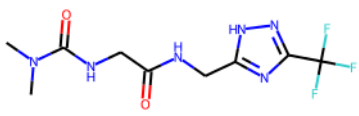
Chemical Structure	SMILES	Vendor
	<chem>CC(=O)N1CCC(NC(=O)C2Cc3cccc3CN2C(C)=O)c2cccc21</chem>	MCULE MCULE-9598391086
	<chem>Cc1ncsc1C(=O)N(C)c1ccccc1C(=O)O</chem>	MCULE MCULE-6998860183
	<chem>Cc1cc(CNC(=O)Cc2ccc(S(N)(=O)=O)s2)n(C)n1</chem>	MCULE MCULE-8017248231

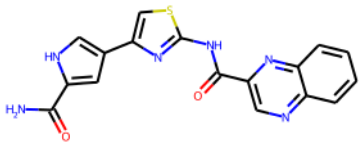
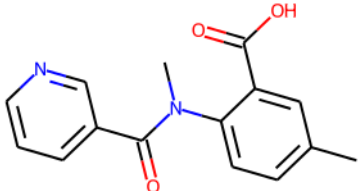
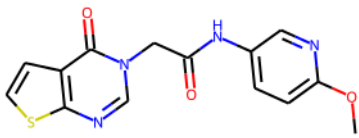
Chemical Structure	SMILES	Vendor
	<chem>Cc1n[nH]c2c1CN(C(=O)c1c3c(nc4cccc14)CCC3)CC2</chem>	MCULE MCULE-2637236638
	<chem>O=C(Nc1c(Cl)ccc2nsnc12)c1cccnc1</chem>	MCULE MCULE-8400791591
	<chem>CN(c1ccc(O)cc1)c1ccc2ncnc1[N+](=O)[O-]</chem>	MCULE MCULE-6628386924

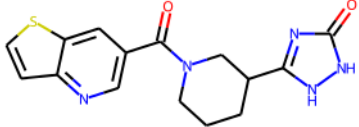
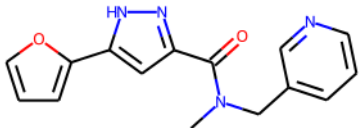
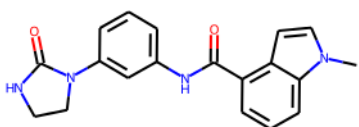
Chemical Structure	SMILES	Vendor
	<chem>Cc1nc2cc(NCc3ccc(O)c3)ccc2n1C</chem>	MCULE MCULE-1578967668
	<chem>CN1CCN(C(=O)c2ccc(NC(=O)CC#N)cc2)CC1</chem>	MCULE MCULE-4607948790
	<chem>CCn1cccc1CNC(=O)c1cc2ncc(Br)cn2n1</chem>	MCULE MCULE-8865818610

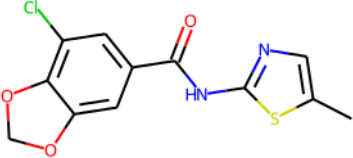
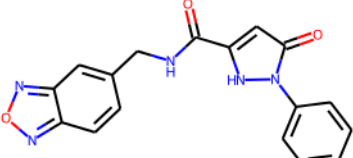

Chemical Structure	SMILES	Vendor
	<chem>Cc1[nH]c2c(C(=O)Nc3nccs3)cccc2c1C</chem>	MCULE MCULE-7167193124
	<chem>CN(CC1CCN(c2ccccc2)C1)C(=O)c1ccc(-n2cnnc2)cc1</chem>	MCULE MCULE-2798708143
	<chem>O=C(CCCn1cccc1)Nc1ccc2nc[nH]c2c1</chem>	MCULE MCULE-5026809838

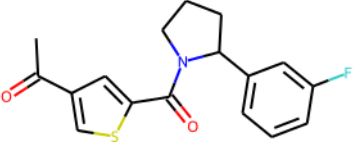
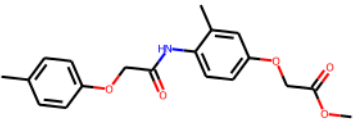
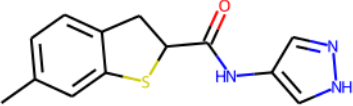
Chemical Structure	SMILES	Vendor
	<chem>N#CCSc1ccc(C(=O)Nc2ccc(-c3nnc[nH]3)cc2)c1</chem>	MCULE MCULE-8914597353
	<chem>O=C(c1ccccc1-c1nnn[nH]1)N(CCCO)Cc1ccc(Cl)cc1</chem>	MCULE MCULE-3692106391
	<chem>Cc1c(C(=O)N(CCC(N)=O)CCc2ccccc2)[nH]c2c(F)cccc12</chem>	MCULE MCULE-3032550299

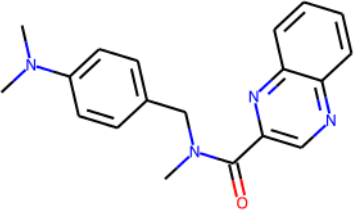
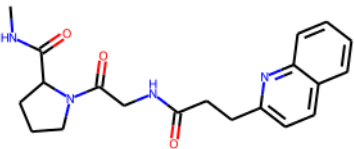
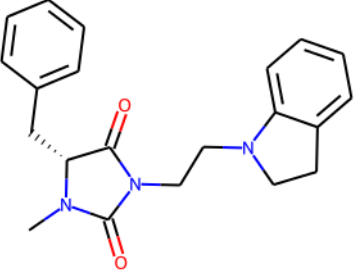
Chemical Structure	SMILES	Vendor
	<chem>O=c1c2sccc2ncn1Cc1csc(-c2ncccn2)n1</chem>	MCULE MCULE-7279167821
	<chem>CC(=O)N1CCc2ccccc2C1</chem> <chem>CC(=O)NC(C(=O)O)c1cccs1</chem>	MCULE MCULE-9599647206
	<chem>CN(C)C(=O)NCC(=O)NCc1nc(C(F)(F)F)n[nH]1</chem>	MCULE MCULE-4061809723

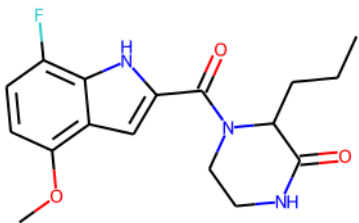
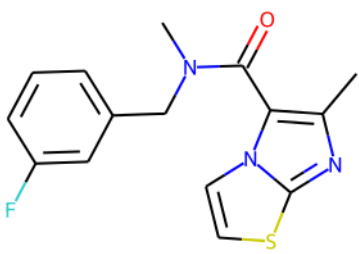
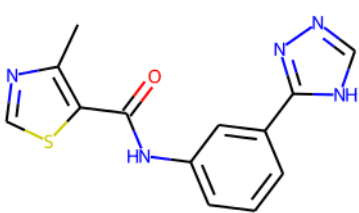
Chemical Structure	SMILES	Vendor
	<chem>NC(=O)c1cc(-c2csc(NC(=O)c3cnc4cccc4n3)n2)c[nH]1</chem>	MCULE MCULE-6470246476
	<chem>Cc1ccc(N(C)C(=O)c2ccncc2)c(C(=O)O)c1</chem>	MCULE MCULE-1470041873
	<chem>COc1ccc(NC(=O)Cn2cnc3sc3c2=O)cn1</chem>	MCULE MCULE-4597697226

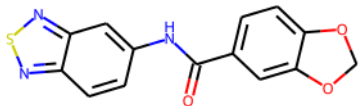
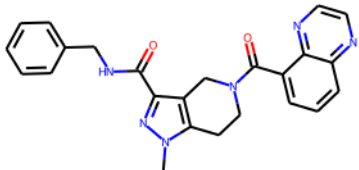
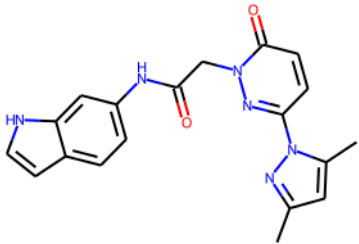
Chemical Structure	SMILES	Vendor
	<chem>O=C(c1cnc2ccsc2c1)N1CCCC(c2nc(=O)[nH][nH]2)C1</chem>	MCULE MCULE-8726891387
	<chem>CN(Cc1cccnc1)C(=O)c1cc(-c2ccco2)[nH]n1</chem>	MCULE MCULE-9075359135
	<chem>Cn1ccc2c(C(=O)Nc3ccc(-c4cccn4)cc3)cccc21</chem>	MCULE MCULE-8676624110

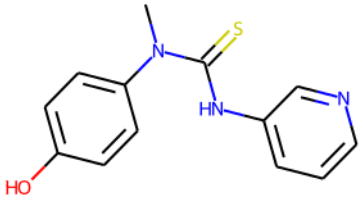
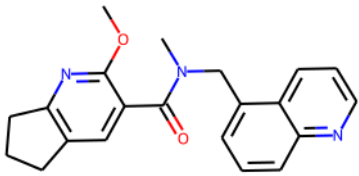
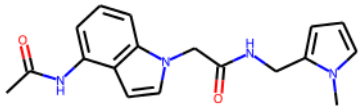
Chemical Structure	SMILES	Vendor
	<chem>Cc1cnc(NC(=O)c2cc(Cl)c3c(c2)OCO3)s1</chem>	MCULE MCULE-7193588229
	<chem>O=C(NCc1ccc2nonc2c1)c1cc(=O)n(-c2ccccc2)[nH]1</chem>	MCULE MCULE-3038738146
	<chem>Cc1c(C(=O)Nc2ncccc2O)oc2c(F)cccc12</chem>	MCULE MCULE-5365829961

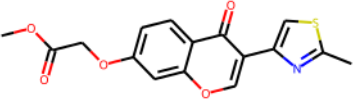
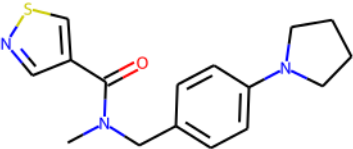
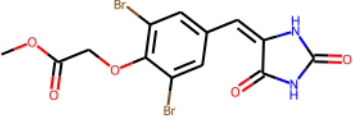
Chemical Structure	SMILES	Vendor
	<chem>CC(=O)c1csc(C(=O)N2C CCC2c2cccc(F)c2)c1</chem>	MCULE MCULE-3757835845
	<chem>COC(=O)COc1ccc(NC(=O))COc2ccc(C)cc2)c(C)c1</chem>	MCULE MCULE-8206073388
	<chem>Cc1ccc2c(c1)SC(C(=O) Nc1cn[nH]c1)C2</chem>	MCULE MCULE-4240201118

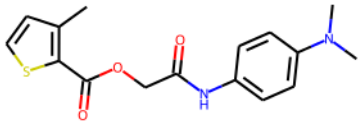
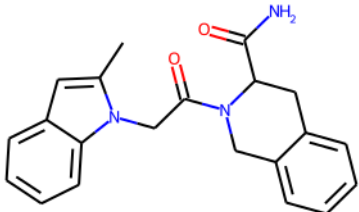
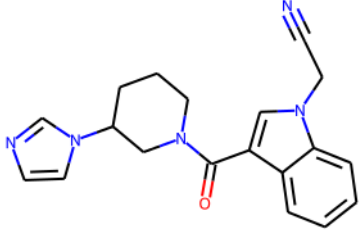
Chemical Structure	SMILES	Vendor
	<chem>CN(Cc1ccc(N(C)C)cc1)C(=O)c1cnc2ccccc2n1</chem>	MCULE MCULE-8689916617
	<chem>CNC(=O)C1CCCN1C(=O)CNC(=O)CCc1ccc2ccccc2n1</chem>	MCULE MCULE-3881000365
	<chem>CN1C(=O)N(CCN2CCc3ccccc32)C(=O)[C@H]1Cc1ccccc1</chem>	MCULE MCULE-7841682728

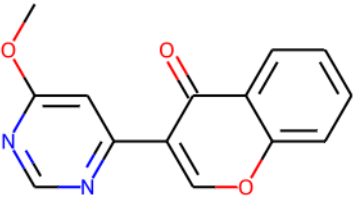
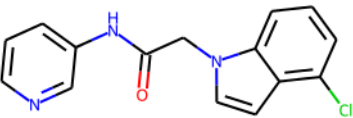
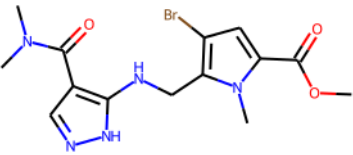
Chemical Structure	SMILES	Vendor
	<chem>CCCC1C(=O)NCCN1C(=O)c1cc2c(OC)ccc(F)c2[nH]1</chem>	MCULE MCULE-5380848690
	<chem>Cc1nc2sccn2c1C(=O)N(C)Cc1cccc(F)c1</chem>	MCULE MCULE-2503164160
	<chem>Cc1ncsc1C(=O)Nc1ccc(-c2nnc[nH]2)c1</chem>	MCULE MCULE-5020445886

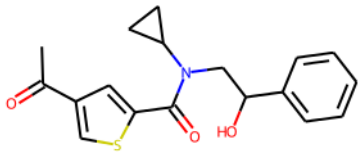
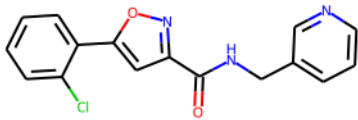
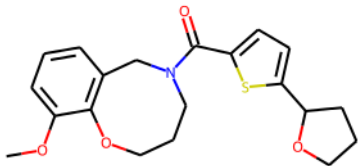
Chemical Structure	SMILES	Vendor
	<chem>O=C(Nc1ccc2nsnc2c1)c1ccc2c(c1)OCO2</chem>	MCULE MCULE-6846089190
	<chem>Cn1nc(C(=O)NCc2ccccc2)c2c1CCN(C(=O)c1cccc3ncnc13)C2</chem>	MCULE MCULE-4252275910
	<chem>Cc1cc(C)n(-c2ccc(=O)n(CC(=O)Nc3ccc4cc[nH]c4c3)n2)n1</chem>	MCULE MCULE-6883299796

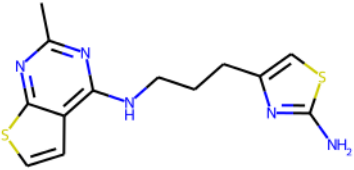
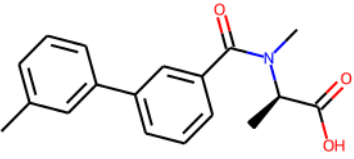
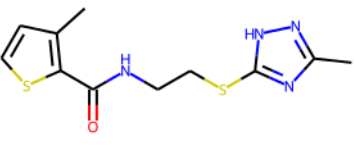
Chemical Structure	SMILES	Vendor
	<chem>CN(C(=S)Nc1cccn1)c1ccc(O)cc1</chem>	MCULE MCULE-1179025630
	<chem>COc1nc2c(cc1C(=O)N(C)Cc1cccc3ncccc13)CCC2</chem>	MCULE MCULE-6954519615
	<chem>CC(=O)Nc1cccc2c1ccn2 CC(=O)NCc1cccn1C</chem>	MCULE MCULE-4584865105

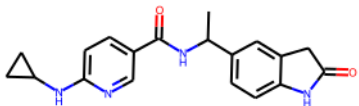
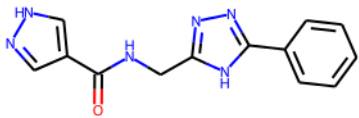
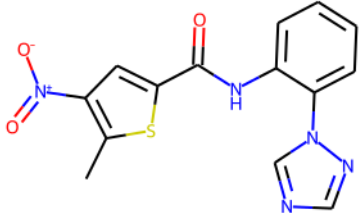
Chemical Structure	SMILES	Vendor
	<chem>COC(=O)COc1ccc2c(=O)c(-c3csc(C)n3)coc2c1</chem>	MCULE MCULE-7648051262
	<chem>CN(Cc1ccc(N2CCCC2)cc1)C(=O)c1cnsc1</chem>	MCULE MCULE-4091995187
	<chem>COC(=O)COc1c(Br)cc(C=C2NC(=O)NC2=O)cc1Br</chem>	MCULE MCULE-2331715829

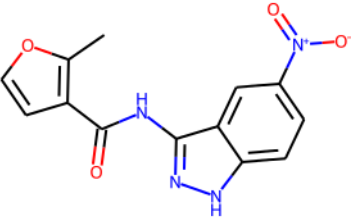
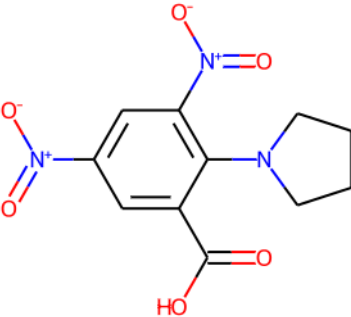
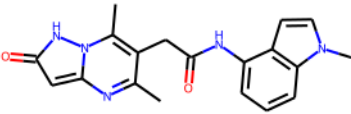
Chemical Structure	SMILES	Vendor
	<chem>Cc1ccsc1C(=O)OCC(=O)Nc1ccc(N(C)C)cc1</chem>	MCULE MCULE-2350134032
	<chem>Cc1cc2ccccc2n1CC(=O)N1Cc2ccccc2CC1C(N)=O</chem>	MCULE MCULE-7151479855
	<chem>N#CCn1cc(C(=O)N2CCCC(n3ccnc3)C2)c2ccccc21</chem>	MCULE MCULE-4062164698

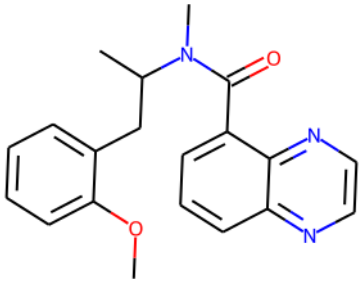
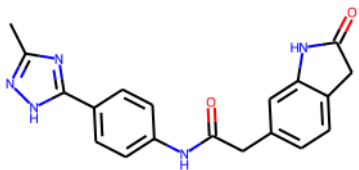
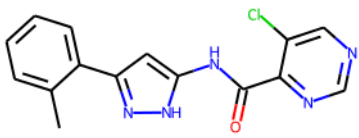
Chemical Structure	SMILES	Vendor
	<chem>COC1CC(-C2COC3CCCCC3C2=O)Ncn1</chem>	MCULE MCULE-4208364355
	<chem>O=C(Cn1ccc2c(Cl)cccc21)Nc1cccnc1</chem>	MCULE MCULE-9500278399
	<chem>COC(=O)c1cc(Br)c(CNc2[nH]ncc2C(=O)N(C)C)n1C</chem>	MCULE MCULE-7413976871

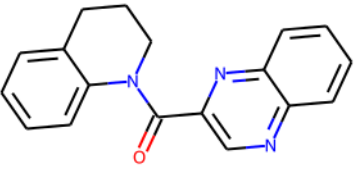
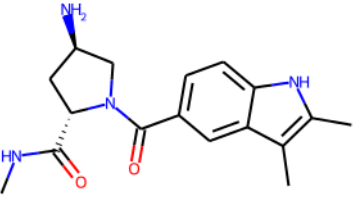
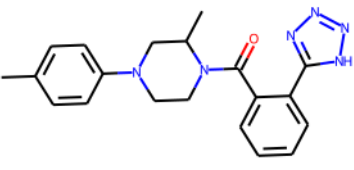
Chemical Structure	SMILES	Vendor
	<chem>CC(=O)c1csc(C(=O)N(C)C(O)c2ccccc2)C2CC2)c1</chem>	MCULE MCULE-6163034620
	<chem>O=C(NCc1ccnc1)c1cc(-c2ccccc2Cl)on1</chem>	MCULE MCULE-6866252827
	<chem>COc1cccc2c1OCCCN(C(=O)c1ccc(C3CCCO3)s1)C2</chem>	MCULE MCULE-3606165410

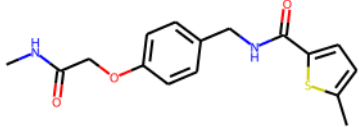
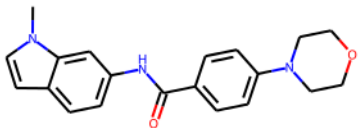
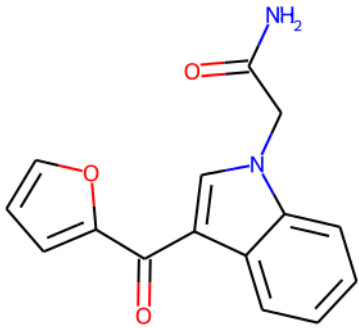
Chemical Structure	SMILES	Vendor
	<chem>Cc1nc(NCCCCc2csc(N)n2)c2ccsc2n1</chem>	MCULE MCULE-3444660335
	<chem>Cc1cccc(-c2cccc(C(=O)N(C)[C@H](C)C(=O)O)c2)c1</chem>	MCULE MCULE-1822258891
	<chem>Cc1n[nH]c(SCCNC(=O)c2sccc2C)n1</chem>	MCULE MCULE-4631088246

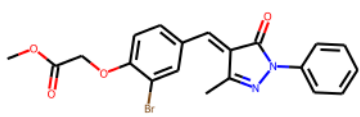
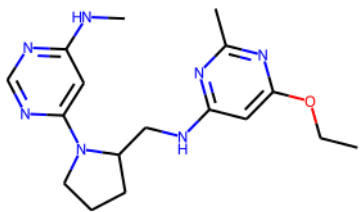
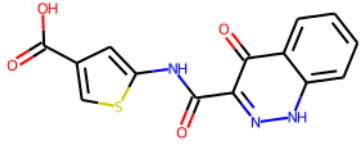
Chemical Structure	SMILES	Vendor
	<chem>CC(NC(=O)c1ccc(NC2CC2)nc1)c1ccc2c(c1)CC(=O)N2</chem>	MCULE MCULE-1046785567
	<chem>O=C(NCc1nnc(-c2ccccc2)[nH]1)c1cn[nH]c1</chem>	MCULE MCULE-7181963692
	<chem>Cc1sc(C(=O)Nc2ccccc2-n2cncn2)cc1[N+](=O)[O-]</chem>	MCULE MCULE-3030740046

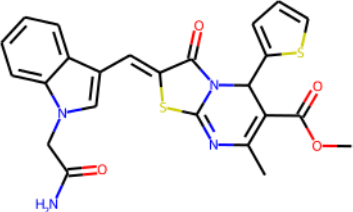
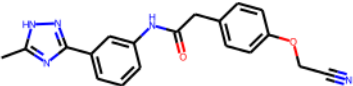
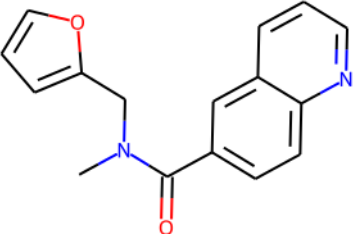
Chemical Structure	SMILES	Vendor
	<chem>Cc1occc1C(=O)Nc1n[nH]c2ccc([N+](=O)[O-])cc12</chem>	MCULE MCULE-9654328112
	<chem>O=C(O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1N1CCCC1</chem>	MCULE MCULE-6082812672
	<chem>Cc1nc2cc(=O)[nH]n2c(C)c1CC(=O)Nc1cccc2c1ccn2C</chem>	MCULE MCULE-3970160208

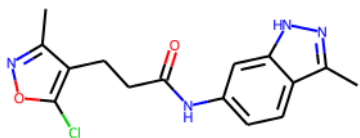
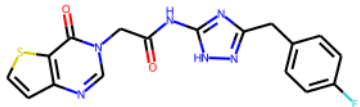
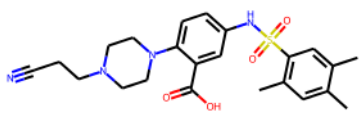
Chemical Structure	SMILES	Vendor
	<chem>COc1ccccc1CC(C)N(C)C(=O)c2ccc2ncnc12</chem>	MCULE MCULE-5061806601
	<chem>Cc1n[nH]c(-c2ccc(NC(=O)Cc3ccc4c(c3)NC(=O)C4)cc2)n1</chem>	MCULE MCULE-8982897524
	<chem>Cc1ccccc1-c1cc(NC(=O)c2ncnc2Cl)[nH]n1</chem>	MCULE MCULE-8656081256

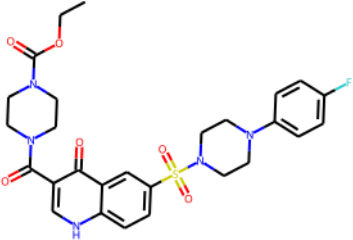
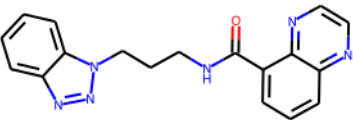
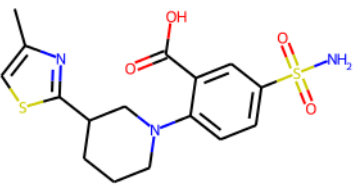
Chemical Structure	SMILES	Vendor
	<chem>O=C(c1cnc2ccccc2n1)N1CCCC2ccccc21</chem>	MCULE MCULE-6931466680
	<chem>CNC(=O)[C@@H]1C[C@@H](N)CN1C(=O)c1ccc2[nH]c(C)c(C)c2c1</chem>	MCULE MCULE-4369706018
	<chem>Cc1ccc(N2CCN(C(=O)c3ccccc3-c3nnn[nH]3)C(C)C2)cc1</chem>	MCULE MCULE-3492289724

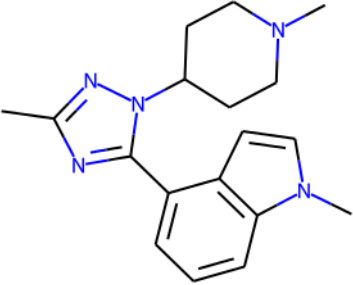
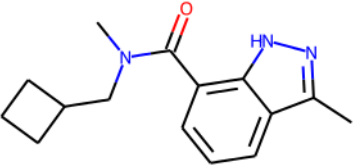
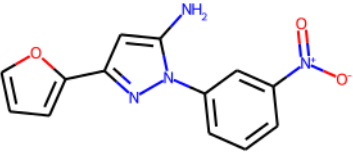
Chemical Structure	SMILES	Vendor
	<chem>CNC(=O)COc1ccc(CNC(=O)c2ccc(C)s2)cc1</chem>	MCULE MCULE-5123696886
	<chem>Cn1ccc2ccc(NC(=O)c3c(N4CCOCC4)cc3)cc21</chem>	MCULE MCULE-1852456739
	<chem>NC(=O)Cn1cc(C(=O)c2c(NC(=O)COc3ccc(CNC(=O)c4ccc(C)s4)cc3)cc21</chem>	MCULE MCULE-3226547122

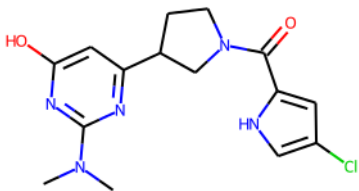
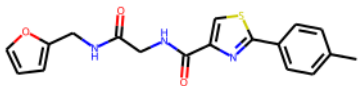
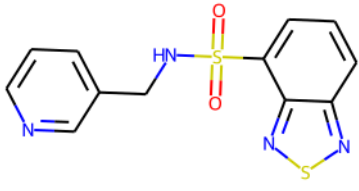
Chemical Structure	SMILES	Vendor
	<chem>COC(=O)COc1ccc(C=C2C(=O)N(c3ccccc3)N=C2C)cc1Br</chem>	MCULE MCULE-5255042277
	<chem>CCOc1cc(NCC2CCCN2c2cnc(NC)nc2)nc(C)n1</chem>	MCULE MCULE-3971409263
	<chem>O=C(O)c1csc(NC(=O)c2c[nH]c3ccccc3c2=O)c1</chem>	MCULE MCULE-4381653735

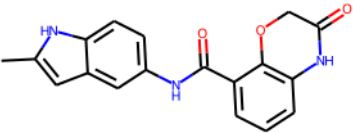
Chemical Structure	SMILES	Vendor
	<chem>COC(=O)C1=C(C)N=c2sc(=Cc3cn(CC(N)=O)c4ccccc34)c(=O)n2C1c1cccs1</chem>	MCULE MCULE-2973639695
	<chem>Cc1nc(-c2cccc(NC(=O)Cc3ccc(OCC#N)cc3)c2)n[nH]1</chem>	MCULE MCULE-7245402730
	<chem>CN(Cc1ccco1)C(=O)c1ccc2ncccc2c1</chem>	MCULE MCULE-1081416350

Chemical Structure	SMILES	Vendor
	<chem>Cc1noc(Cl)c1CCC(=O)N</chem> <chem>c1ccc2c(C)n[nH]c2c1</chem>	MCULE MCULE-6119140869
	<chem>O=C(Cn1cnc2ccsc2c1=O)</chem> <chem>Nc1nc(Cc2ccc(F)cc2)n[nH]1</chem>	MCULE MCULE-9002113746
	<chem>Cc1cc(C)c(S(=O)(=O)N</chem> <chem>c2ccc(N3CCN(CCC#N)CC</chem> <chem>3)c(C(=O)O)c2cc1C</chem>	MCULE MCULE-2443974746

Chemical Structure	SMILES	Vendor
	<chem>CCOC(=O)N1CCN(C(=O)c2c[nH]c3ccc(S(=O)(=O)N4CCN(c5ccc(F)cc5)C(C4)cc3c2=O)CC1</chem>	MCULE MCULE-8830940744
	<chem>O=C(NCCCN1nnc2ccccc21)c1cccc2nccnc12</chem>	MCULE MCULE-4992727916
	<chem>Cc1csc(C2CCCN(c3ccc(S(N)(=O)=O)cc3C(=O)O)C2)n1</chem>	MCULE MCULE-3843127860

Chemical Structure	SMILES	Vendor
	<chem>Cc1nc(-c2cccc3c2ccn3C)n(C2CCN(C)CC2)n1</chem>	MCULE MCULE-8109956160
	<chem>Cc1n[nH]c2c(C(=O)N(C)CC3CCCC3)cccc12</chem>	MCULE MCULE-4818373206
	<chem>Nc1cc(-c2ccco2)nn1-c1cccc([N+](=O)[O-])c1</chem>	MCULE MCULE-7312425133

Chemical Structure	SMILES	Vendor
	<chem>CN(C)c1nc(O)cc(C2CCN(C(=O)c3cc(Cl)c[nH]3)C2)n1</chem>	MCULE MCULE-2406359046
	<chem>Cc1ccc(-c2nc(C(=O)NC(=O)NCc3ccco3)cs2)cc1</chem>	MCULE MCULE-1504229129
	<chem>O=S(=O)(NCc1cccnc1)c1cccc2nsnc12</chem>	MCULE MCULE-2054108963

Chemical Structure	SMILES	Vendor
	<chem>Cc1cc2cc(NC(=O)c3ccc4c3OCC(=O)N4)ccc2[nH]1</chem>	MCULE MCULE-3705422053